Parameter Performance

Variables testing

formula = class ~ B1

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
37.09	49.06	16.98

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	17	5	0	***	SIPr&BA	4	18	0
SIPr	12	9	0	***	SIPr	16	5	0
TAC	6	4	0	***	TAC	4	6	0

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
45.28%	0.014

Variable Importance

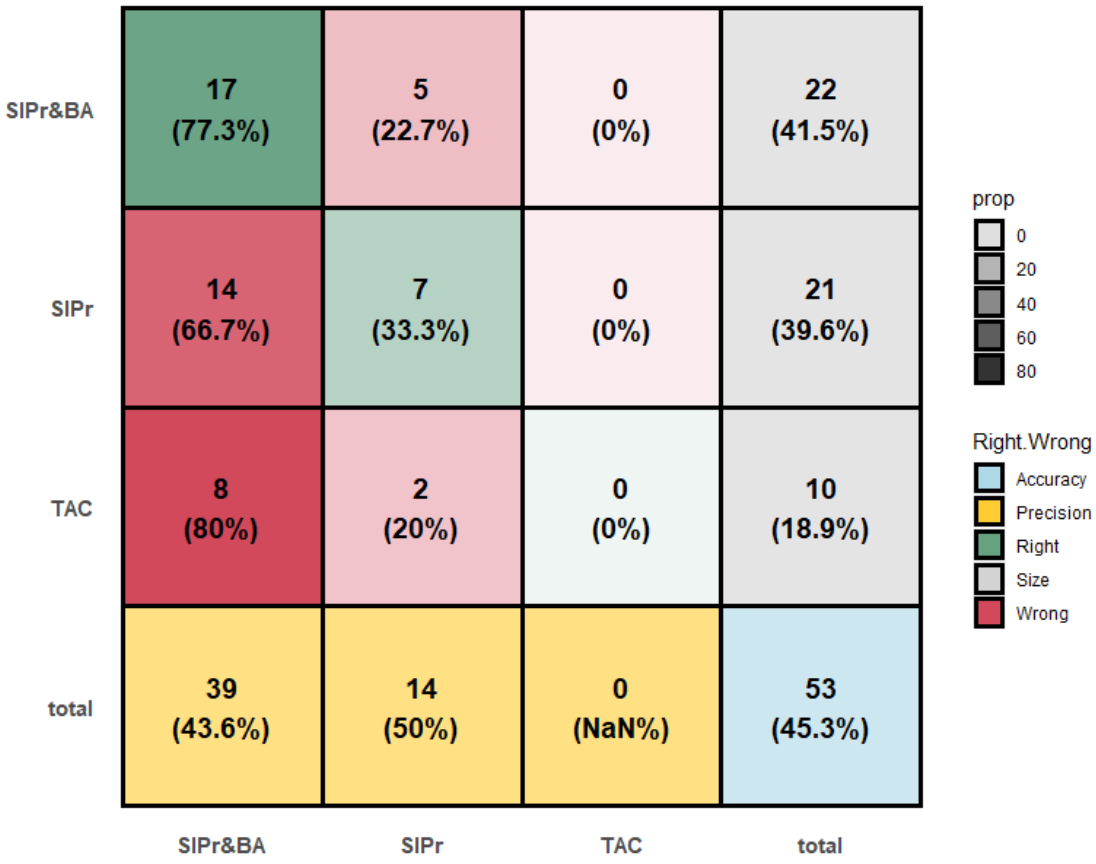
	Overall
B1	0.4094161

Coefficients

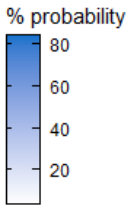
	(Intercept)	B1
2	-0.0488632	0.3697058
3	-0.7941191	-0.0397103

exp(coefficients)

	(Intercept)	B1
2	0.9523114	1.4473087
3	0.4519792	0.9610678


SIPr&BA
SIPr
TAC
total
17 (77.3%)
5 (22.7%)
0 (0%)
22 (41.5%)
14 (66.7%)
7 (33.3%)
0 (0%)
21 (39.6%)
8 (80%)
2 (20%)
0 (0%)
10 (18.9%)
39 (43.6%)
14 (50%)
0 (NaN%)
53 (45.3%)
SIPr&BA
SIPr
TAC
total
prop
0
20
40
60
80
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	45	34	21	SIPr&BA
3-Br	43	37	20	SIPr&BA
3-Cl	44	35	21	SIPr&BA
3-CN	45	34	21	SIPr&BA
3-F	45	34	21	SIPr&BA
3-I	42	40	19	SIPr&BA
3-CO2Me	44	35	20	SIPr&BA
3-CF3	39	44	17	SIPr&BA
4-Br	38	45	17	SIPr&BA
4-Cl	42	38	19	SIPr&BA
4-CN	45	34	21	SIPr&BA
4-F	45	34	21	SIPr&BA
4-I	31	56	13	SIPr&BA
4-CO2Me	42	39	19	SIPr&BA
4-CF3	32	55	14	SIPr&BA
3,5-Br	38	45	17	SIPr&BA
3,5-Cl	42	38	19	SIPr&BA
6a	44	35	21	SIPr&BA
6b	45	34	21	SIPr&BA
6c	45	34	21	SIPr&BA
6d	43	37	20	SIPr&BA
6e	45	34	21	SIPr&BA
2-Br	43	37	20	SIPr
2-Cl	44	35	21	SIPr
2-C=CH	45	34	21	SIPr
2-OH	45	34	21	SIPr
2-Ome	44	36	20	SIPr
2-Me	44	36	20	SIPr
2-CF3	38	45	17	SIPr
2-OCF3	40	42	18	SIPr
3-Me	44	36	20	SIPr
3-Ome	43	37	20	SIPr
4-CH(OEt)2	11	84	4	SIPr
4-iPr	34	51	15	SIPr
4-Ome	43	37	20	SIPr
4-Me	42	39	19	SIPr
6f	35	50	15	SIPr
6g	45	34	21	SIPr
6h	43	38	19	SIPr
6i	34	51	15	SIPr
6j	44	35	20	SIPr
6k	39	44	17	SIPr
6l	45	34	21	SIPr
6m	36	49	16	TAC
6n	44	36	20	TAC
6o	41	40	19	TAC
6p	41	40	19	TAC
6q	45	34	21	TAC
6r	45	34	21	TAC
6s	40	42	18	TAC
6t	44	36	20	TAC
6u	45	34	21	TAC
6v	42	39	19	TAC



formula = class ~ C=O

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
63.36	69.81	49.06

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	18	3	1	***	SIPr&BA	17	3	2
SIPr	6	14	1	***	SIPr	15	3	3
TAC	0	5	5	***	TAC	0	4	6

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
67.92%	0.316

Variable Importance

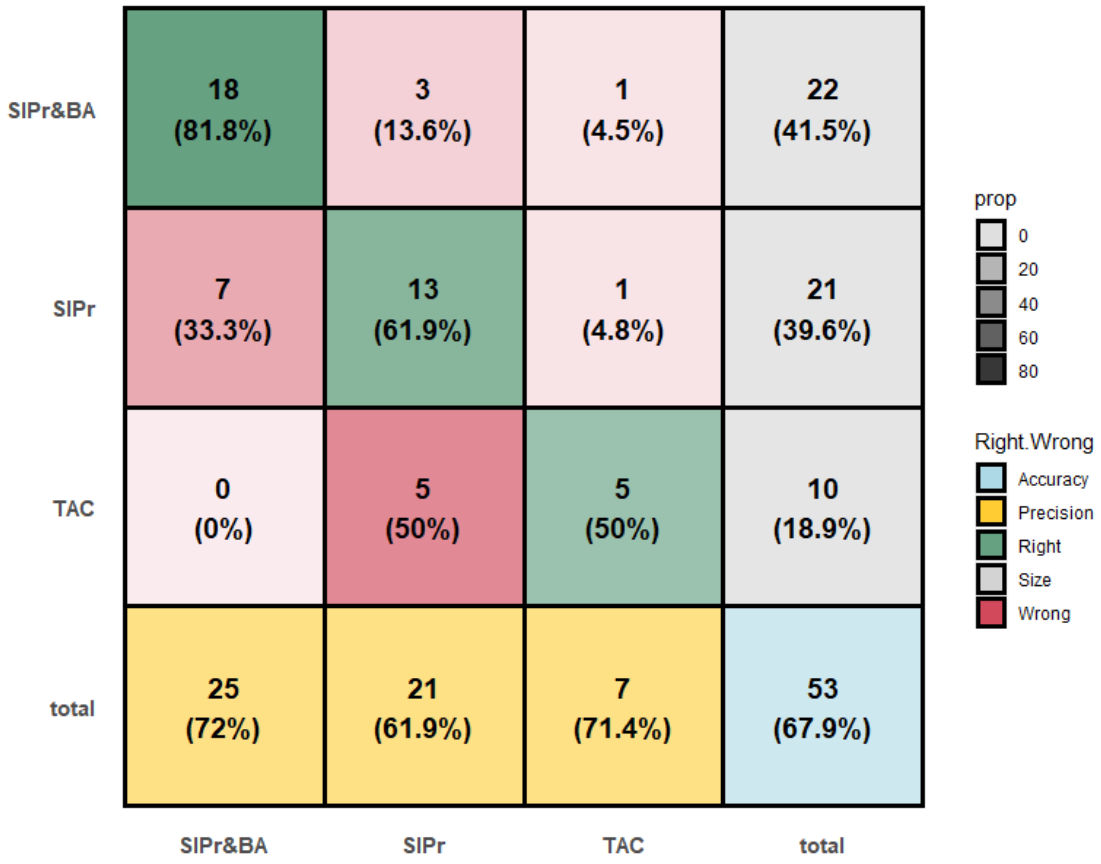
	Overall
C.O	5.600699

Coefficients

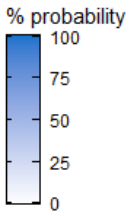
	(Intercept)	C.O
2	0.5194145	-1.664868
3	-1.6302255	-3.935831

exp(coefficients)

	(Intercept)	C.O
2	1.6810431	0.1892157
3	0.1958854	0.0195295


SIPr&BA
SIPr
TAC
total
18 (81.8%)
3 (13.6%)
1 (4.5%)
22 (41.5%)
7 (33.3%)
13 (61.9%)
1 (4.8%)
21 (39.6%)
0 (0%)
5 (50%)
5 (50%)
10 (18.9%)
25 (72%)
21 (61.9%)
7 (71.4%)
53 (67.9%)
SIPr&BA
SIPr
TAC
total
prop
0
20
40
60
80
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	26	62	12	SIPr&BA
3-Br	73	26	0	SIPr&BA
3-Cl	73	26	0	SIPr&BA
3-CN	81	19	0	SIPr&BA
3-F	75	25	0	SIPr&BA
3-I	72	27	0	SIPr&BA
3-CO2Me	66	34	1	SIPr&BA
3-CF3	76	23	0	SIPr&BA
4-Br	61	38	1	SIPr&BA
4-Cl	59	39	1	SIPr&BA
4-CN	79	21	0	SIPr&BA
4-F	55	43	2	SIPr&BA
4-I	60	39	1	SIPr&BA
4-CO2Me	71	29	0	SIPr&BA
4-CF3	79	21	0	SIPr&BA
3,5-Br	82	18	0	SIPr&BA
3,5-Cl	82	18	0	SIPr&BA
6a	67	32	1	SIPr&BA
6b	47	50	3	SIPr&BA
6c	8	53	38	SIPr&BA
6d	68	32	1	SIPr&BA
6e	3	33	64	SIPr&BA
2-Br	25	63	13	SIPr
2-Cl	23	63	14	SIPr
2-C=CH	31	61	9	SIPr
2-OH	7	50	44	SIPr
2-Ome	3	38	58	SIPr
2-Me	6	47	47	SIPr
2-CF3	42	54	4	SIPr
2-OCF3	22	63	15	SIPr
3-Me	55	43	2	SIPr
3-Ome	63	36	1	SIPr
4-CH(OEt)2	55	43	2	SIPr
4-iPr	40	55	5	SIPr
4-Ome	21	63	16	SIPr
4-Me	43	53	4	SIPr
6f	78	22	0	SIPr
6g	23	63	14	SIPr
6h	67	33	1	SIPr
6i	64	35	1	SIPr
6j	22	63	15	SIPr
6k	66	34	1	SIPr
6l	7	49	44	SIPr
6m	10	56	34	TAC
6n	2	33	65	TAC
6o	26	62	12	TAC
6p	2	30	68	TAC
6q	14	60	26	TAC
6r	8	53	39	TAC
6s	11	58	30	TAC
6t	0	7	93	TAC
6u	0	0	100	TAC
6v	0	3	97	TAC



formula = class ~ L

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
32.56	47.17	15.09

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	16	5	1	***	SIPr&BA	6	16	0
SIPr	13	8	0	***	SIPr	19	2	0
TAC	6	3	1	***	TAC	6	4	0

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
39.62%	0.023

Variable Importance

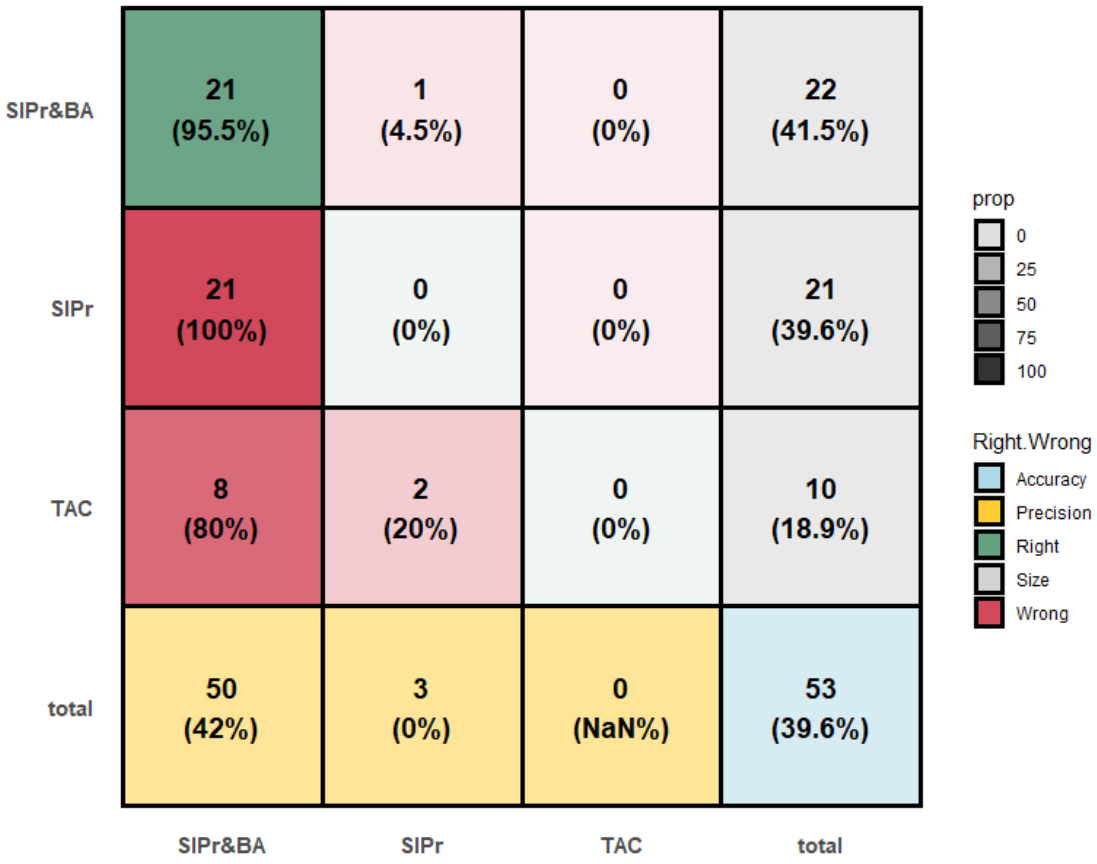
	Overall
L	0.9113633

Coefficients

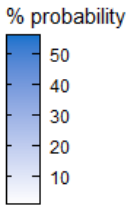
	(Intercept)	L
2	-0.0416231	-0.0565049
3	-0.9522087	-0.8548585

exp(coefficients)

	(Intercept)	L
2	0.9592313	0.9450619
3	0.3858878	0.4253434


SIPr&BA
SIPr
TAC
total
21 (95.5%)
1 (4.5%)
0 (0%)
22 (41.5%)
21 (100%)
0 (0%)
0 (0%)
21 (39.6%)
8 (80%)
2 (20%)
0 (0%)
10 (18.9%)
50 (42%)
3 (0%)
0 (NaN%)
53 (39.6%)
SIPr&BA
SIPr
TAC
total
prop
0
25
50
75
100
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	38	38	24	SIPr&BA
3-Br	38	38	24	SIPr&BA
3-Cl	38	38	24	SIPr&BA
3-CN	39	38	23	SIPr&BA
3-F	38	38	24	SIPr&BA
3-I	40	39	21	SIPr&BA
3-CO2Me	45	42	12	SIPr&BA
3-CF3	39	38	23	SIPr&BA
4-Br	45	42	13	SIPr&BA
4-Cl	44	41	15	SIPr&BA
4-CN	46	43	11	SIPr&BA
4-F	40	39	20	SIPr&BA
4-I	46	43	12	SIPr&BA
4-CO2Me	48	44	9	SIPr&BA
4-CF3	43	41	16	SIPr&BA
3,5-Br	39	38	23	SIPr&BA
3,5-Cl	38	38	24	SIPr&BA
6a	56	43	1	SIPr&BA
6b	39	38	23	SIPr&BA
6c	45	42	13	SIPr&BA
6d	52	44	3	SIPr&BA
6e	35	36	29	SIPr&BA
2-Br	38	38	24	SIPr
2-Cl	38	38	24	SIPr
2-C=CH	38	38	24	SIPr
2-OH	38	38	24	SIPr
2-Ome	38	38	24	SIPr
2-Me	38	38	24	SIPr
2-CF3	38	38	24	SIPr
2-OCF3	38	38	24	SIPr
3-Me	38	38	24	SIPr
3-Ome	41	40	19	SIPr
4-CH(OEt)2	47	43	10	SIPr
4-iPr	46	43	11	SIPr
4-Ome	46	43	12	SIPr
4-Me	42	40	18	SIPr
6f	54	44	2	SIPr
6g	38	38	24	SIPr
6h	51	44	5	SIPr
6i	40	39	21	SIPr
6j	38	38	24	SIPr
6k	53	44	2	SIPr
6l	39	38	23	SIPr
6m	38	38	24	TAC
6n	38	38	24	TAC
6o	38	38	24	TAC
6p	38	38	24	TAC
6q	38	38	24	TAC
6r	45	43	12	TAC
6s	48	44	8	TAC
6t	34	35	31	TAC
6u	35	35	30	TAC
6v	40	39	21	TAC



formula = class ~ position

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
45.8	54.72	26.42

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	18	4	0	***	SIPr&BA	11	7	4
SIPr	10	11	0	***	SIPr	10	1	10
TAC	1	9	0	***	TAC	1	7	2

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
54.72%	0.158

Variable Importance

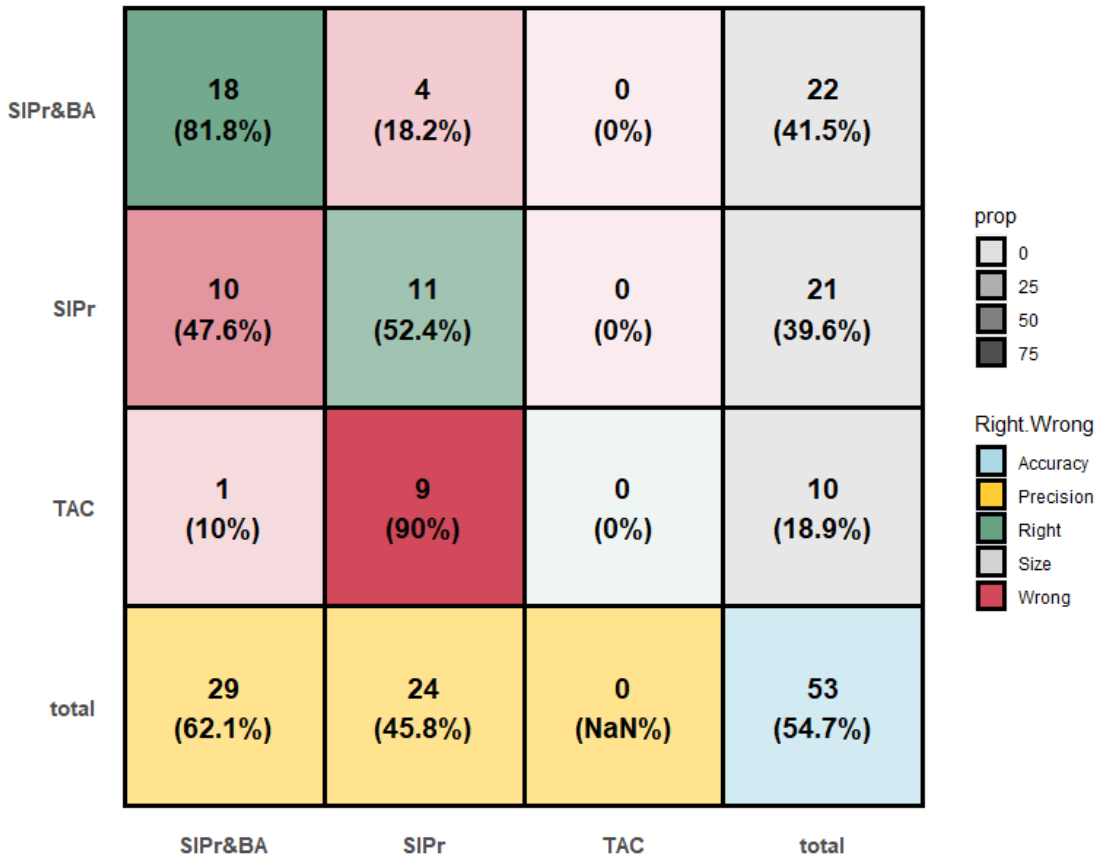
	Overall
position3	4.826276
position4	13.639297

Coefficients

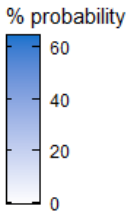
	(Intercept)	position3	position4
2	1.0115015	-1.617567	-1.571117
3	0.8108966	-3.208710	-12.068181

exp(coefficients)

	(Intercept)	position3	position4
2	2.749727	0.1983808	0.2078130
3	2.249924	0.0404087	0.0000057


SIPr&BA
SIPr
TAC
total
18 (81.8%)
4 (18.2%)
0 (0%)
22 (41.5%)
10 (47.6%)
11 (52.4%)
0 (0%)
21 (39.6%)
1 (10%)
9 (90%)
0 (0%)
10 (18.9%)
29 (62.1%)
24 (45.8%)
0 (NaN%)
53 (54.7%)
SIPr&BA
SIPr
TAC
total
prop
0
25
50
75
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	17	46	38	SIPr&BA
3-Br	61	33	6	SIPr&BA
3-Cl	61	33	6	SIPr&BA
3-CN	61	33	6	SIPr&BA
3-F	61	33	6	SIPr&BA
3-I	61	33	6	SIPr&BA
3-CO2Me	61	33	6	SIPr&BA
3-CF3	61	33	6	SIPr&BA
4-Br	64	36	0	SIPr&BA
4-Cl	64	36	0	SIPr&BA
4-CN	64	36	0	SIPr&BA
4-F	64	36	0	SIPr&BA
4-I	64	36	0	SIPr&BA
4-CO2Me	64	36	0	SIPr&BA
4-CF3	64	36	0	SIPr&BA
3,5-Br	61	33	6	SIPr&BA
3,5-Cl	61	33	6	SIPr&BA
6a	61	33	6	SIPr&BA
6b	17	46	38	SIPr&BA
6c	17	46	38	SIPr&BA
6d	61	33	6	SIPr&BA
6e	17	46	38	SIPr&BA
2-Br	17	46	38	SIPr
2-Cl	17	46	38	SIPr
2-C=CH	17	46	38	SIPr
2-OH	17	46	38	SIPr
2-Ome	17	46	38	SIPr
2-Me	17	46	38	SIPr
2-CF3	17	46	38	SIPr
2-OCF3	17	46	38	SIPr
3-Me	61	33	6	SIPr
3-Ome	61	33	6	SIPr
4-CH(OEt)2	64	36	0	SIPr
4-iPr	64	36	0	SIPr
4-Ome	64	36	0	SIPr
4-Me	64	36	0	SIPr
6f	61	33	6	SIPr
6g	17	46	38	SIPr
6h	61	33	6	SIPr
6i	61	33	6	SIPr
6j	17	46	38	SIPr
6k	61	33	6	SIPr
6l	17	46	38	SIPr
6m	17	46	38	TAC
6n	17	46	38	TAC
6o	17	46	38	TAC
6p	17	46	38	TAC
6q	17	46	38	TAC
6r	17	46	38	TAC
6s	61	33	6	TAC
6t	17	46	38	TAC
6u	17	46	38	TAC
6v	17	46	38	TAC



formula = class ~ NBO_Carbonyl

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
36.2	52.83	18.87

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	18	2	2	***	SIPr&BA	6	14	2
SIPr	13	8	0	***	SIPr	18	3	0
TAC	5	3	2	***	TAC	4	5	1

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
41.51%	0.073

Variable Importance

	Overall
NBO_Carbonyl	1.028487

Coefficients

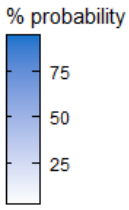
	(Intercept)	NBO_Carbonyl
2	-0.0386392	-0.0383765
3	-0.9463336	-0.9901103

exp(coefficients)

	(Intercept)	NBO_Carbonyl
2	0.9620978	0.9623505
3	0.3881616	0.3715357


SIPr&BA
SIPr
TAC
total
20 (90.9%)
0 (0%)
2 (9.1%)
22 (41.5%)
21 (100%)
0 (0%)
0 (0%)
21 (39.6%)
8 (80%)
0 (0%)
2 (20%)
10 (18.9%)
49 (40.8%)
0 (NaN%)
4 (50%)
53 (41.5%)
SIPr&BA
SIPr
TAC
total
prop
0
25
50
75
100
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	40	39	21	SIPr&BA
3-Br	47	44	10	SIPr&BA
3-Cl	46	44	10	SIPr&BA
3-CN	46	43	11	SIPr&BA
3-F	46	43	11	SIPr&BA
3-I	47	44	9	SIPr&BA
3-CO2Me	47	44	10	SIPr&BA
3-CF3	46	43	11	SIPr&BA
4-Br	46	43	11	SIPr&BA
4-Cl	46	43	11	SIPr&BA
4-CN	44	42	15	SIPr&BA
4-F	46	44	10	SIPr&BA
4-I	46	43	11	SIPr&BA
4-CO2Me	45	42	13	SIPr&BA
4-CF3	45	43	12	SIPr&BA
3,5-Br	47	44	9	SIPr&BA
3,5-Cl	46	44	10	SIPr&BA
6a	46	44	10	SIPr&BA
6b	39	38	23	SIPr&BA
6c	20	21	59	SIPr&BA
6d	47	44	9	SIPr&BA
6e	20	21	59	SIPr&BA
2-Br	42	40	18	SIPr
2-Cl	41	40	20	SIPr
2-C=CH	38	37	24	SIPr
2-OH	40	39	21	SIPr
2-Ome	41	40	20	SIPr
2-Me	42	41	17	SIPr
2-CF3	36	35	29	SIPr
2-OCF3	40	39	21	SIPr
3-Me	47	44	9	SIPr
3-Ome	47	44	9	SIPr
4-CH(OEt)2	46	44	10	SIPr
4-iPr	47	44	9	SIPr
4-Ome	46	43	10	SIPr
4-Me	46	44	10	SIPr
6f	46	43	10	SIPr
6g	45	43	13	SIPr
6h	47	44	10	SIPr
6i	48	44	8	SIPr
6j	42	41	17	SIPr
6k	47	44	10	SIPr
6l	41	40	19	SIPr
6m	34	34	32	TAC
6n	41	40	20	TAC
6o	43	41	16	TAC
6p	41	39	20	TAC
6q	46	43	11	TAC
6r	42	41	17	TAC
6s	46	43	10	TAC
6t	3	3	94	TAC
6u	10	10	80	TAC
6v	34	34	32	TAC



formula = class ~ diff_Ca_O

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
52.89	64.15	30.19

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	17	5	0	***	SIPr&BA	5	17	0
SIPr	6	15	0	***	SIPr	7	11	3
TAC	3	5	2	***	TAC	2	8	0

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
60.38%	0.109

Variable Importance

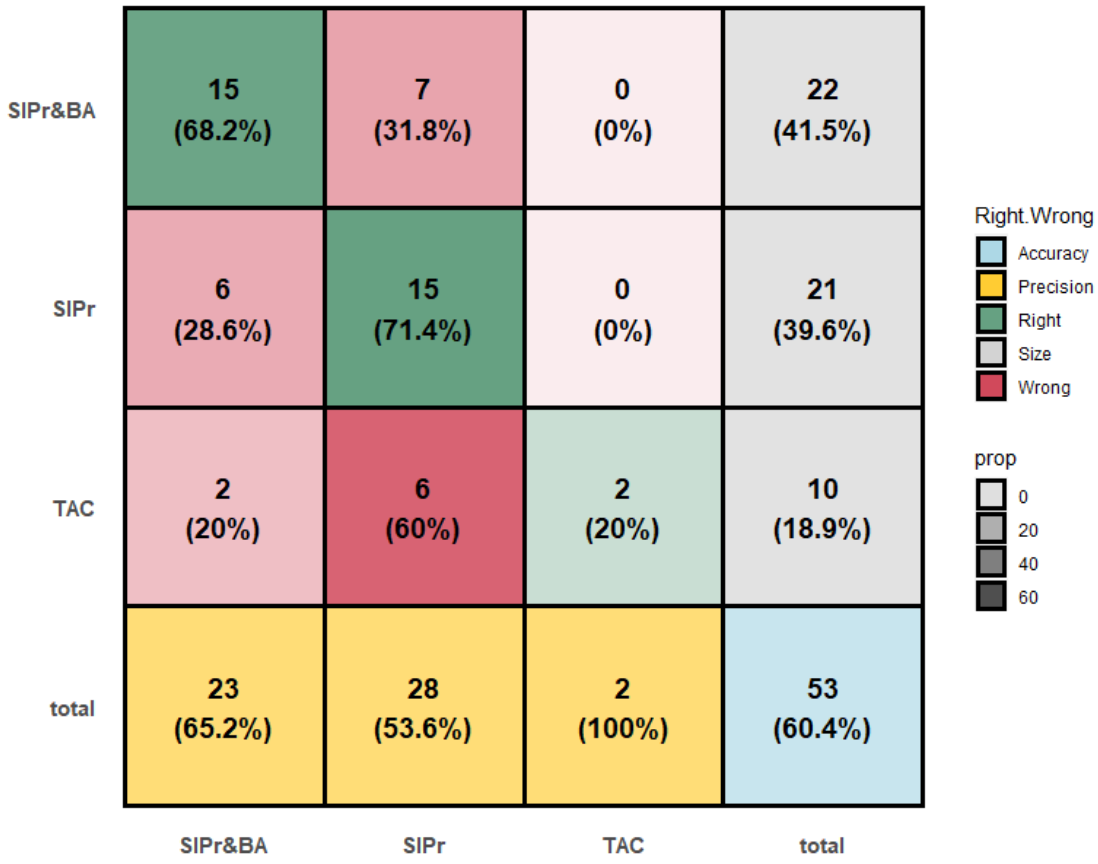
	Overall
diff_Ca_O	2.496464

Coefficients

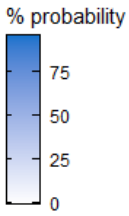
	(Intercept)	diff_Ca_O
2	0.0638037	0.9983671
3	-0.8864903	1.4980966

exp(coefficients)

	(Intercept)	diff_Ca_O
2	1.0658832	2.713847
3	0.4120996	4.473167


SIPr&BA
SIPr
TAC
total
15 (68.2%)
7 (31.8%)
0 (0%)
22 (41.5%)
6 (28.6%)
15 (71.4%)
0 (0%)
21 (39.6%)
2 (20%)
6 (60%)
2 (20%)
10 (18.9%)
23 (65.2%)
28 (53.6%)
2 (100%)
53 (60.4%)
SIPr&BA
SIPr
TAC
total
Right.Wrong
Accuracy
Precision
Right
Size
Wrong
prop
0
20
40
60

	SIPr&BA	SIPr	TAC	Exp
2-F	52	37	12	SIPr&BA
3-Br	47	40	14	SIPr&BA
3-Cl	46	40	14	SIPr&BA
3-CN	63	30	8	SIPr&BA
3-F	49	38	13	SIPr&BA
3-I	44	41	15	SIPr&BA
3-CO2Me	34	46	20	SIPr&BA
3-CF3	52	36	11	SIPr&BA
4-Br	39	44	18	SIPr&BA
4-Cl	36	45	19	SIPr&BA
4-CN	74	22	4	SIPr&BA
4-F	24	49	26	SIPr&BA
4-I	39	44	17	SIPr&BA
4-CO2Me	56	34	10	SIPr&BA
4-CF3	61	31	8	SIPr&BA
3,5-Br	66	28	7	SIPr&BA
3,5-Cl	65	28	7	SIPr&BA
6a	42	42	16	SIPr&BA
6b	81	16	3	SIPr&BA
6c	89	10	1	SIPr&BA
6d	38	44	18	SIPr&BA
6e	74	22	4	SIPr&BA
2-Br	55	34	10	SIPr
2-Cl	55	35	10	SIPr
2-C=CH	54	35	11	SIPr
2-OH	23	50	27	SIPr
2-Ome	19	50	31	SIPr
2-Me	24	49	27	SIPr
2-CF3	76	20	4	SIPr
2-OCF3	56	34	10	SIPr
3-Me	22	50	28	SIPr
3-Ome	28	48	24	SIPr
4-CH(OEt)2	27	49	24	SIPr
4-iPr	16	50	34	SIPr
4-Ome	8	48	44	SIPr
4-Me	17	50	33	SIPr
6f	51	37	12	SIPr
6g	39	44	17	SIPr
6h	39	44	18	SIPr
6i	29	48	23	SIPr
6j	39	44	17	SIPr
6k	35	45	19	SIPr
6l	32	47	21	SIPr
6m	39	44	17	TAC
6n	16	50	33	TAC
6o	54	35	11	TAC
6p	16	50	34	TAC
6q	16	50	34	TAC
6r	28	48	24	TAC
6s	5	45	50	TAC
6t	95	5	0	TAC
6u	12	50	38	TAC
6v	5	44	51	TAC



formula = class ~ Tot

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
51.28	64.15	35.85

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	16	6	0	***	SIPr&BA	14	7	1
SIPr	6	14	1	***	SIPr	13	5	3
TAC	3	3	4	***	TAC	1	9	0

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
52.83%	0.145

Variable Importance

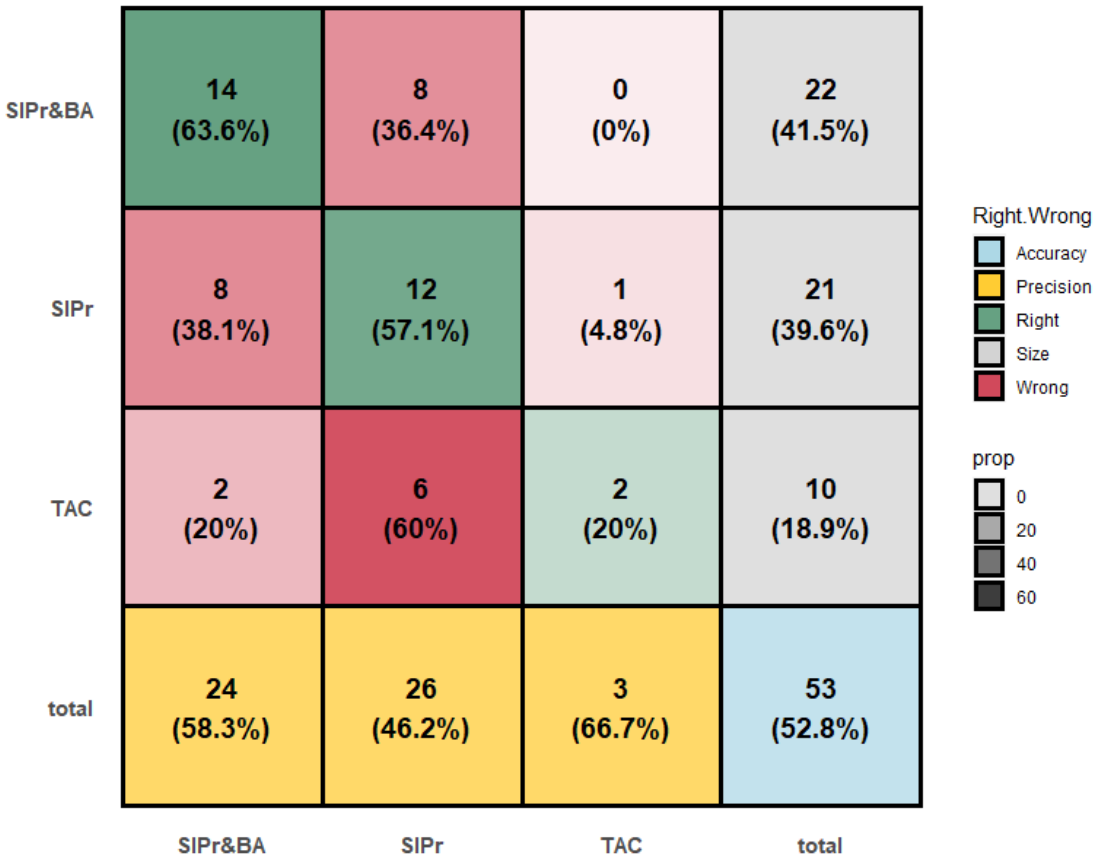
	Overall
Tot	2.993127

Coefficients

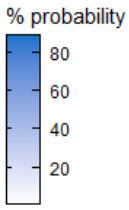
	(Intercept)	Tot
2	0.1580898	1.130233
3	-0.9300456	1.862893

exp(coefficients)

	(Intercept)	Tot
2	1.1712714	3.096379
3	0.3945357	6.442350


SIPr&BA
SIPr
TAC
total
14 (63.6%)
8 (36.4%)
0 (0%)
22 (41.5%)
8 (38.1%)
12 (57.1%)
1 (4.8%)
21 (39.6%)
2 (20%)
6 (60%)
2 (20%)
10 (18.9%)
24 (58.3%)
26 (46.2%)
3 (66.7%)
53 (52.8%)
SIPr&BA
SIPr
TAC
total
Right.Wrong
Accuracy
Precision
Right
Size
Wrong
prop
0
20
40
60

	SIPr&BA	SIPr	TAC	Exp
2-F	34	48	18	SIPr&BA
3-Br	60	33	7	SIPr&BA
3-Cl	68	28	5	SIPr&BA
3-CN	88	11	1	SIPr&BA
3-F	85	13	1	SIPr&BA
3-I	42	44	14	SIPr&BA
3-CO2Me	37	46	16	SIPr&BA
3-CF3	89	11	1	SIPr&BA
4-Br	54	37	9	SIPr&BA
4-Cl	59	34	7	SIPr&BA
4-CN	71	25	4	SIPr&BA
4-F	72	24	4	SIPr&BA
4-I	39	46	15	SIPr&BA
4-CO2Me	26	50	23	SIPr&BA
4-CF3	68	28	5	SIPr&BA
3,5-Br	57	35	8	SIPr&BA
3,5-Cl	63	31	6	SIPr&BA
6a	27	50	23	SIPr&BA
6b	62	32	6	SIPr&BA
6c	28	50	22	SIPr&BA
6d	12	50	38	SIPr&BA
6e	60	33	7	SIPr&BA
2-Br	49	40	11	SIPr
2-Cl	48	41	11	SIPr
2-C=CH	44	43	13	SIPr
2-OH	14	50	36	SIPr
2-Ome	9	48	43	SIPr
2-Me	36	47	17	SIPr
2-CF3	29	50	21	SIPr
2-OCF3	43	44	13	SIPr
3-Me	33	48	19	SIPr
3-Ome	22	51	27	SIPr
4-CH(OEt)2	87	12	1	SIPr
4-iPr	31	49	20	SIPr
4-Ome	52	38	10	SIPr
4-Me	33	48	19	SIPr
6f	1	23	76	SIPr
6g	64	30	6	SIPr
6h	17	51	31	SIPr
6i	25	51	24	SIPr
6j	49	40	11	SIPr
6k	50	40	10	SIPr
6l	36	47	17	SIPr
6m	38	46	16	TAC
6n	8	47	44	TAC
6o	45	43	13	TAC
6p	8	47	44	TAC
6q	9	48	43	TAC
6r	41	45	14	TAC
6s	7	46	47	TAC
6t	9	48	42	TAC
6u	58	35	8	TAC
6v	5	43	52	TAC



formula = class ~ B5

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
44.67	56.6	26.42

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	17	5	0	***	SIPr&BA	7	13	2
SIPr	8	13	0	***	SIPr	12	7	2
TAC	4	6	0	***	TAC	0	10	0

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
52.83%	0.053

Variable Importance

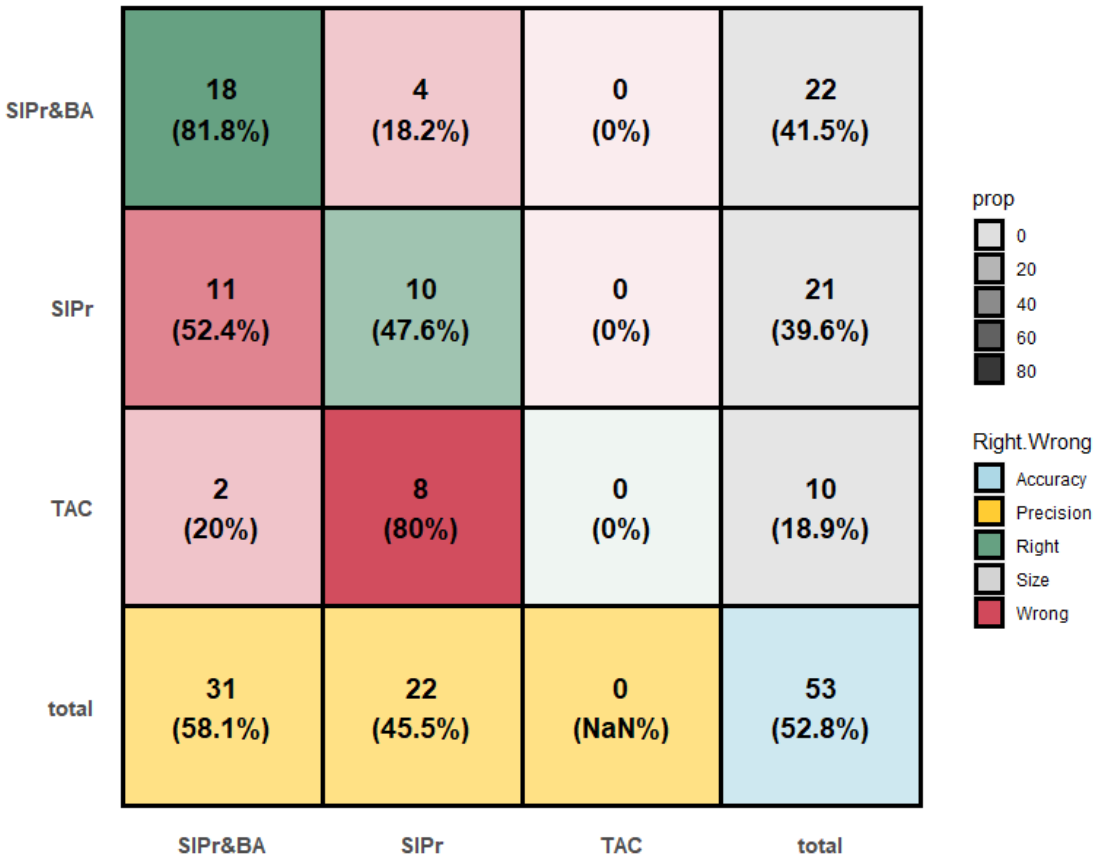
	Overall
B5	1.783978

Coefficients

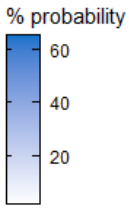
	(Intercept)	B5
2	0.0592936	0.8816097
3	-0.6879984	0.9023683

exp(coefficients)

	(Intercept)	B5
2	1.061087	2.414784
3	0.502581	2.465435


SIPr&BA
SIPr
TAC
total
18 (81.8%)
4 (18.2%)
0 (0%)
22 (41.5%)
11 (52.4%)
10 (47.6%)
0 (0%)
21 (39.6%)
2 (20%)
8 (80%)
0 (0%)
10 (18.9%)
31 (58.1%)
22 (45.5%)
0 (NaN%)
53 (52.8%)
SIPr&BA
SIPr
TAC
total
prop
0
20
40
60
80
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	55	31	14	SIPr&BA
3-Br	45	38	18	SIPr&BA
3-Cl	47	36	17	SIPr&BA
3-CN	42	40	19	SIPr&BA
3-F	54	31	15	SIPr&BA
3-I	41	40	19	SIPr&BA
3-CO2Me	40	41	19	SIPr&BA
3-CF3	44	38	18	SIPr&BA
4-Br	59	28	13	SIPr&BA
4-Cl	59	28	13	SIPr&BA
4-CN	59	28	13	SIPr&BA
4-F	59	28	13	SIPr&BA
4-I	59	28	13	SIPr&BA
4-CO2Me	58	28	13	SIPr&BA
4-CF3	59	28	13	SIPr&BA
3,5-Br	45	38	18	SIPr&BA
3,5-Cl	47	36	17	SIPr&BA
6a	7	62	31	SIPr&BA
6b	38	42	20	SIPr&BA
6c	55	31	14	SIPr&BA
6d	20	54	26	SIPr&BA
6e	60	27	13	SIPr&BA
2-Br	44	38	18	SIPr
2-Cl	47	36	17	SIPr
2-C=CH	38	42	20	SIPr
2-OH	51	33	16	SIPr
2-Ome	40	41	19	SIPr
2-Me	50	34	16	SIPr
2-CF3	44	38	18	SIPr
2-OCF3	36	43	21	SIPr
3-Me	48	35	17	SIPr
3-Ome	46	36	17	SIPr
4-CH(OEt)2	39	41	19	SIPr
4-iPr	59	28	13	SIPr
4-Ome	59	28	13	SIPr
4-Me	59	28	13	SIPr
6f	2	65	33	SIPr
6g	24	52	25	SIPr
6h	19	54	26	SIPr
6i	9	61	30	SIPr
6j	43	39	18	SIPr
6k	5	63	32	SIPr
6l	38	42	20	SIPr
6m	26	50	24	TAC
6n	14	58	28	TAC
6o	41	40	19	TAC
6p	29	48	23	TAC
6q	40	41	19	TAC
6r	38	42	20	TAC
6s	31	46	22	TAC
6t	25	51	24	TAC
6u	60	27	13	TAC
6v	40	41	19	TAC



Models

formula = class ~ C=O + position

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
60.97	71.7	45.28

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	19	2	1	***	SIPr&BA	9	12	1
SIPr	6	14	1	***	SIPr	9	10	2
TAC	1	4	5	***	TAC	0	5	5

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
71.7%	0.341

Variable Importance

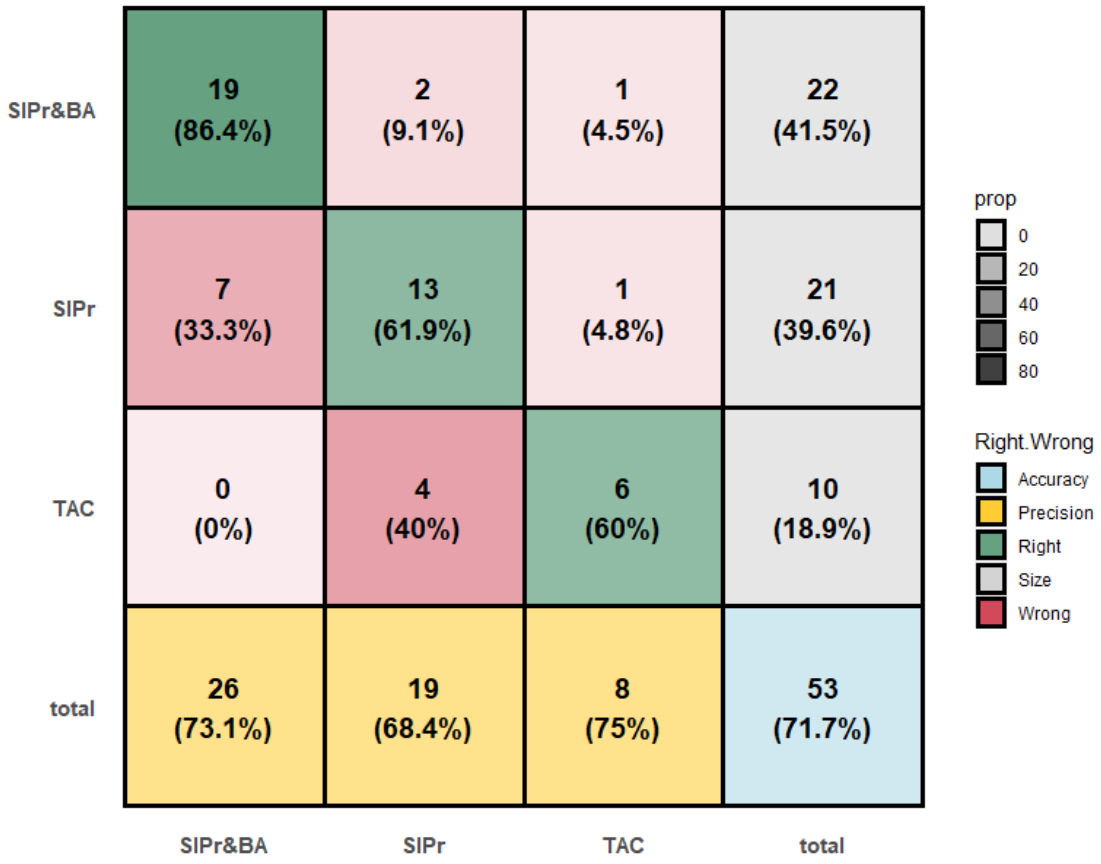
	Overall
C.O	7.460110
position3	4.188149
position4	7.229402

Coefficients

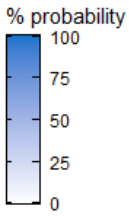
	(Intercept)	C.O	position3	position4
2	0.1371464	-2.516607	1.379799	0.5005251
3	-2.2253181	-4.943504	2.808349	-6.7288770

exp(coefficients)

	(Intercept)	C.O	position3	position4
2	1.146996	0.0807331	3.974105	1.6495872
3	0.108033	0.0071296	16.582526	0.0011959


SIPr&BA
SIPr
TAC
total
19 (86.4%)
2 (9.1%)
1 (4.5%)
22 (41.5%)
7 (33.3%)
13 (61.9%)
1 (4.8%)
21 (39.6%)
0 (0%)
4 (40%)
6 (60%)
10 (18.9%)
26 (73.1%)
19 (68.4%)
8 (75%)
53 (71.7%)
SIPr&BA
SIPr
TAC
total
prop
0
20
40
60
80
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	30	60	10	SIPr&BA
3-Br	68	30	1	SIPr&BA
3-Cl	69	30	1	SIPr&BA
3-CN	81	19	0	SIPr&BA
3-F	71	28	1	SIPr&BA
3-I	67	32	1	SIPr&BA
3-CO2Me	55	42	3	SIPr&BA
3-CF3	74	25	1	SIPr&BA
4-Br	71	29	0	SIPr&BA
4-Cl	68	32	0	SIPr&BA
4-CN	90	10	0	SIPr&BA
4-F	62	38	0	SIPr&BA
4-I	69	31	0	SIPr&BA
4-CO2Me	82	18	0	SIPr&BA
4-CF3	89	11	0	SIPr&BA
3,5-Br	82	17	0	SIPr&BA
3,5-Cl	83	17	0	SIPr&BA
6a	58	39	2	SIPr&BA
6b	62	36	2	SIPr&BA
6c	7	57	37	SIPr&BA
6d	59	39	2	SIPr&BA
6e	1	34	65	SIPr&BA
2-Br	29	61	10	SIPr
2-Cl	26	62	12	SIPr
2-C=CH	38	55	7	SIPr
2-OH	5	52	43	SIPr
2-Ome	2	40	58	SIPr
2-Me	4	50	46	SIPr
2-CF3	55	43	3	SIPr
2-OCF3	25	63	13	SIPr
3-Me	38	55	7	SIPr
3-Ome	51	45	4	SIPr
4-CH(OEt)2	63	37	0	SIPr
4-iPr	41	59	0	SIPr
4-Ome	18	82	0	SIPr
4-Me	46	54	0	SIPr
6f	76	23	1	SIPr
6g	26	62	12	SIPr
6h	57	40	3	SIPr
6i	53	44	3	SIPr
6j	24	63	13	SIPr
6k	55	42	3	SIPr
6l	5	52	44	SIPr
6m	8	59	32	TAC
6n	1	34	65	TAC
6o	31	60	9	TAC
6p	1	30	69	TAC
6q	13	63	24	TAC
6r	6	56	38	TAC
6s	1	33	65	TAC
6t	0	6	94	TAC
6u	0	0	100	TAC
6v	0	3	97	TAC



formula = class ~ C=O + position + Tot

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
60.11	73.58	39.62

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	18	3	1	***	SIPr&BA	8	13	1
SIPr	3	16	2	***	SIPr	9	8	4
TAC	0	5	5	***	TAC	0	5	5

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
77.36%	0.388

Variable Importance

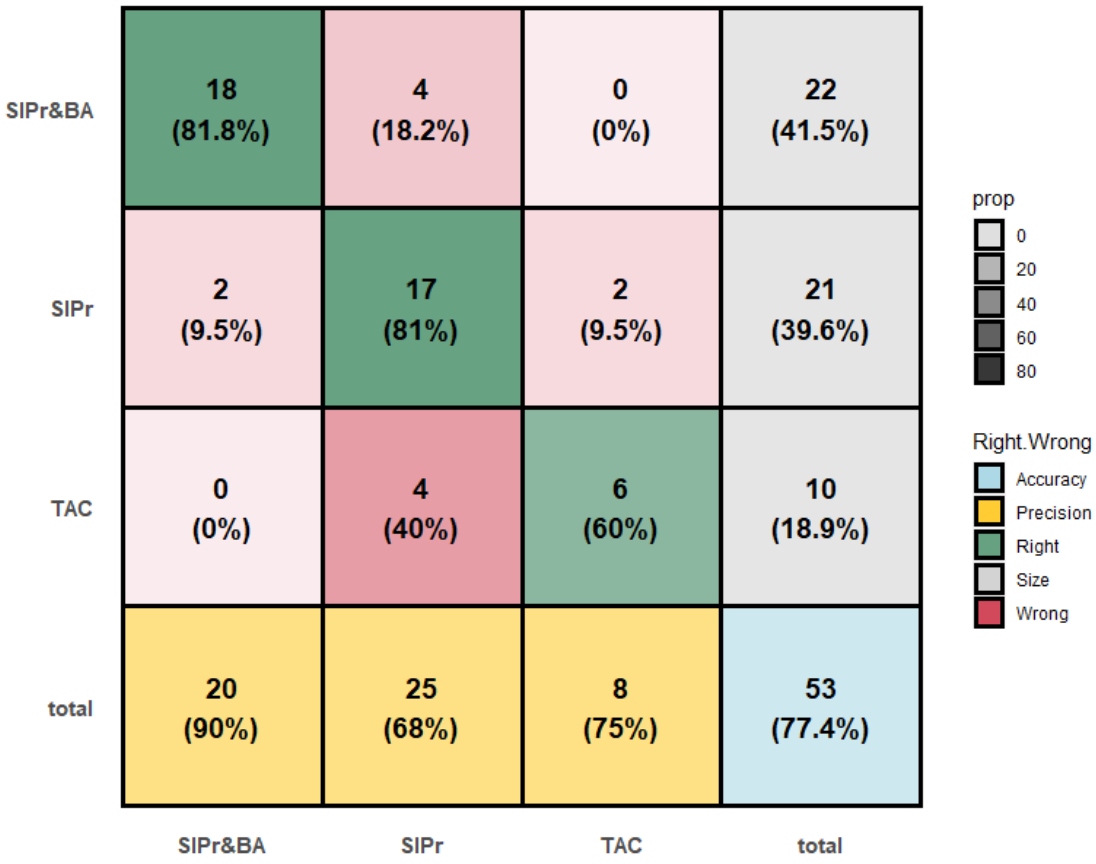
	Overall
C.O	6.092577
position3	1.725928
position4	7.990051
Tot	2.469160

Coefficients

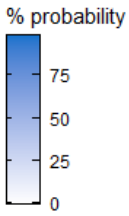
	(Intercept)	C.O	position3	position4	Tot
2	0.4014782	-2.031821	0.6241651	0.3824734	0.8696894
3	-1.9286358	-4.060757	1.1017631	-7.6075778	1.5994703

exp(coefficients)

	(Intercept)	C.O	position3	position4	Tot
2	1.4940316	0.1310966	1.866687	1.4659058	2.38617
3	0.1453463	0.0172360	3.009467	0.0004967	4.95041


SIPr&BA
SIPr
TAC
total
18 (81.8%)
4 (18.2%)
0 (0%)
22 (41.5%)
2 (9.5%)
17 (81%)
2 (9.5%)
21 (39.6%)
0 (0%)
4 (40%)
6 (60%)
10 (18.9%)
20 (90%)
25 (68%)
8 (75%)
53 (77.4%)
SIPr&BA
SIPr
TAC
total
prop
0
20
40
60
80
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	24	65	11	SIPr&BA
3-Br	80	19	0	SIPr&BA
3-Cl	84	16	0	SIPr&BA
3-CN	96	4	0	SIPr&BA
3-F	92	8	0	SIPr&BA
3-I	70	29	1	SIPr&BA
3-CO2Me	58	40	2	SIPr&BA
3-CF3	94	6	0	SIPr&BA
4-Br	70	30	0	SIPr&BA
4-Cl	71	29	0	SIPr&BA
4-CN	92	8	0	SIPr&BA
4-F	75	25	0	SIPr&BA
4-I	60	40	0	SIPr&BA
4-CO2Me	64	36	0	SIPr&BA
4-CF3	91	9	0	SIPr&BA
3,5-Br	87	12	0	SIPr&BA
3,5-Cl	89	11	0	SIPr&BA
6a	53	45	2	SIPr&BA
6b	68	31	1	SIPr&BA
6c	5	57	37	SIPr&BA
6d	38	58	4	SIPr&BA
6e	5	54	40	SIPr&BA
2-Br	32	60	8	SIPr
2-Cl	29	62	9	SIPr
2-C=CH	36	58	6	SIPr
2-OH	2	44	54	SIPr
2-Ome	1	28	71	SIPr
2-Me	5	55	40	SIPr
2-CF3	39	56	5	SIPr
2-OCF3	25	64	11	SIPr
3-Me	42	54	4	SIPr
3-Ome	43	54	4	SIPr
4-CH(OEt)2	86	14	0	SIPr
4-iPr	31	69	0	SIPr
4-Ome	24	76	0	SIPr
4-Me	37	63	0	SIPr
6f	15	72	12	SIPr
6g	41	54	5	SIPr
6h	43	54	3	SIPr
6i	47	50	3	SIPr
6j	28	62	9	SIPr
6k	67	32	1	SIPr
6l	6	57	37	SIPr
6m	9	63	27	TAC
6n	0	23	77	TAC
6o	31	61	8	TAC
6p	0	21	79	TAC
6q	3	53	44	TAC
6r	8	62	30	TAC
6s	1	35	64	TAC
6t	0	6	94	TAC
6u	0	2	98	TAC
6v	0	2	98	TAC



formula = class ~ C=O + position + Tot + L

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
59.47	73.58	39.62

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	17	2	3	***	SIPr&BA	11	10	1
SIPr	2	17	2	***	SIPr	13	4	4
TAC	0	5	5	***	TAC	1	3	6

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
77.36%	0.389

Variable Importance

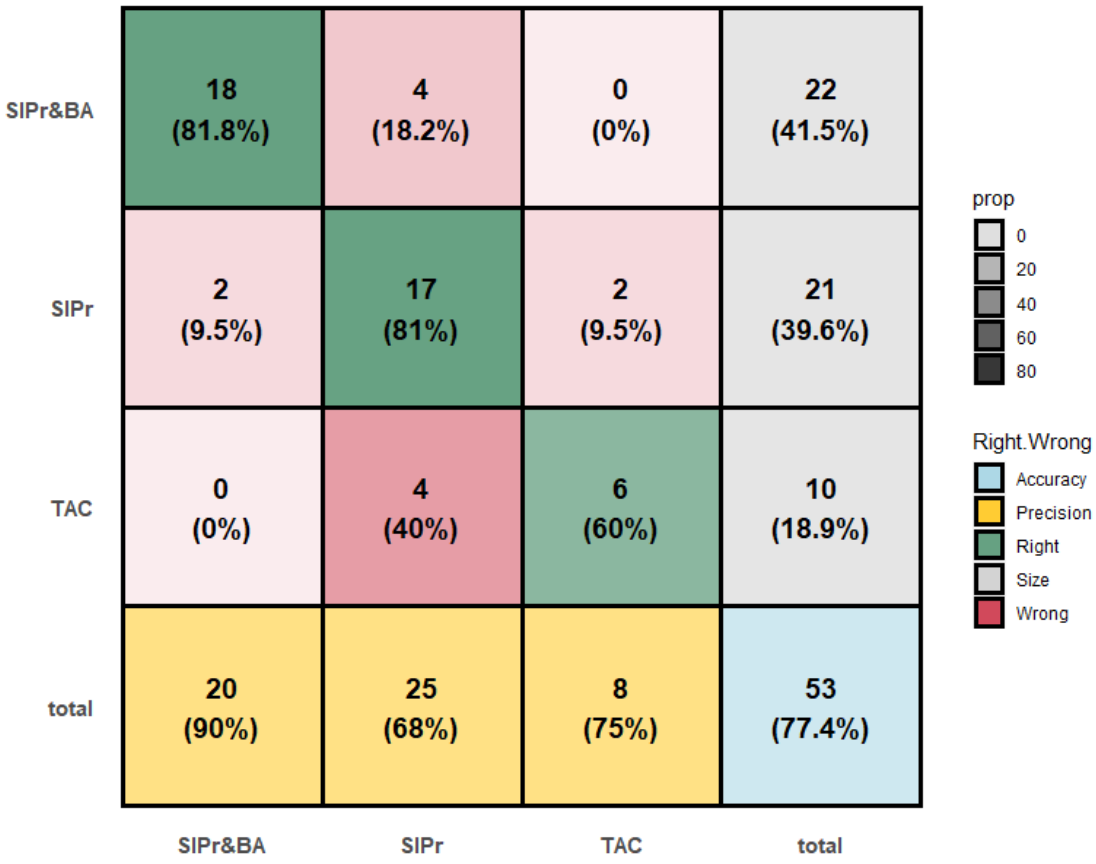
	Overall
C.O	6.1324932
position3	1.6568118
position4	10.9116071
Tot	2.5830804
L	0.2552311

Coefficients

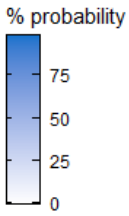
	(Intercept)	C.O	position3	position4	Tot	L
2	0.3476996	-2.006292	0.7475414	0.5032132	0.9557541	-0.1474682
3	-1.9164033	-4.126201	0.9092704	-10.4083940	1.6273263	0.1077629

exp(coefficients)

	(Intercept)	C.O	position3	position4	Tot	L
2	1.4158069	0.1344864	2.111802	1.6540274	2.600631	0.8628898
3	0.1471352	0.0161441	2.482511	0.0000302	5.090247	1.1137836


SIPr&BA
SIPr
TAC
total
18 (81.8%)
4 (18.2%)
0 (0%)
22 (41.5%)
2 (9.5%)
17 (81%)
2 (9.5%)
21 (39.6%)
0 (0%)
4 (40%)
6 (60%)
10 (18.9%)
20 (90%)
25 (68%)
8 (75%)
53 (77.4%)
SIPr&BA
SIPr
TAC
total
prop
0
20
40
60
80
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	24	66	10	SIPr&BA
3-Br	79	21	0	SIPr&BA
3-Cl	83	17	0	SIPr&BA
3-CN	96	4	0	SIPr&BA
3-F	92	8	0	SIPr&BA
3-I	67	32	1	SIPr&BA
3-CO2Me	58	41	1	SIPr&BA
3-CF3	94	6	0	SIPr&BA
4-Br	70	30	0	SIPr&BA
4-Cl	71	29	0	SIPr&BA
4-CN	92	8	0	SIPr&BA
4-F	74	26	0	SIPr&BA
4-I	60	40	0	SIPr&BA
4-CO2Me	64	36	0	SIPr&BA
4-CF3	91	9	0	SIPr&BA
3,5-Br	86	14	0	SIPr&BA
3,5-Cl	88	12	0	SIPr&BA
6a	62	35	3	SIPr&BA
6b	69	30	1	SIPr&BA
6c	6	53	42	SIPr&BA
6d	40	55	5	SIPr&BA
6e	5	55	40	SIPr&BA
2-Br	32	61	7	SIPr
2-Cl	29	62	8	SIPr
2-C=CH	36	58	6	SIPr
2-OH	2	45	53	SIPr
2-Ome	1	29	70	SIPr
2-Me	5	56	39	SIPr
2-CF3	37	58	5	SIPr
2-OCF3	25	64	10	SIPr
3-Me	38	60	3	SIPr
3-Ome	39	59	3	SIPr
4-CH(OEt)2	88	12	0	SIPr
4-iPr	31	69	0	SIPr
4-Ome	25	75	0	SIPr
4-Me	34	66	0	SIPr
6f	16	69	15	SIPr
6g	42	53	5	SIPr
6h	45	51	3	SIPr
6i	43	55	2	SIPr
6j	29	62	9	SIPr
6k	73	26	1	SIPr
6l	6	57	37	SIPr
6m	9	64	27	TAC
6n	0	24	76	TAC
6o	31	61	8	TAC
6p	0	21	78	TAC
6q	3	56	41	TAC
6r	9	56	35	TAC
6s	1	36	63	TAC
6t	0	6	94	TAC
6u	0	2	98	TAC
6v	0	2	98	TAC



formula = class ~ C=O + position + Tot + L + B5

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
66.69	79.25	50.94

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	21	1	0	***	SIPr&BA	13	7	2
SIPr	3	17	1	***	SIPr	5	10	6
TAC	0	6	4	***	TAC	0	6	4

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
90.57%	0.819

Variable Importance

	Overall
C.O	539.4211
position3	374.5238
position4	908.7111
Tot	359.6741
L	707.6875
B5	1081.9934

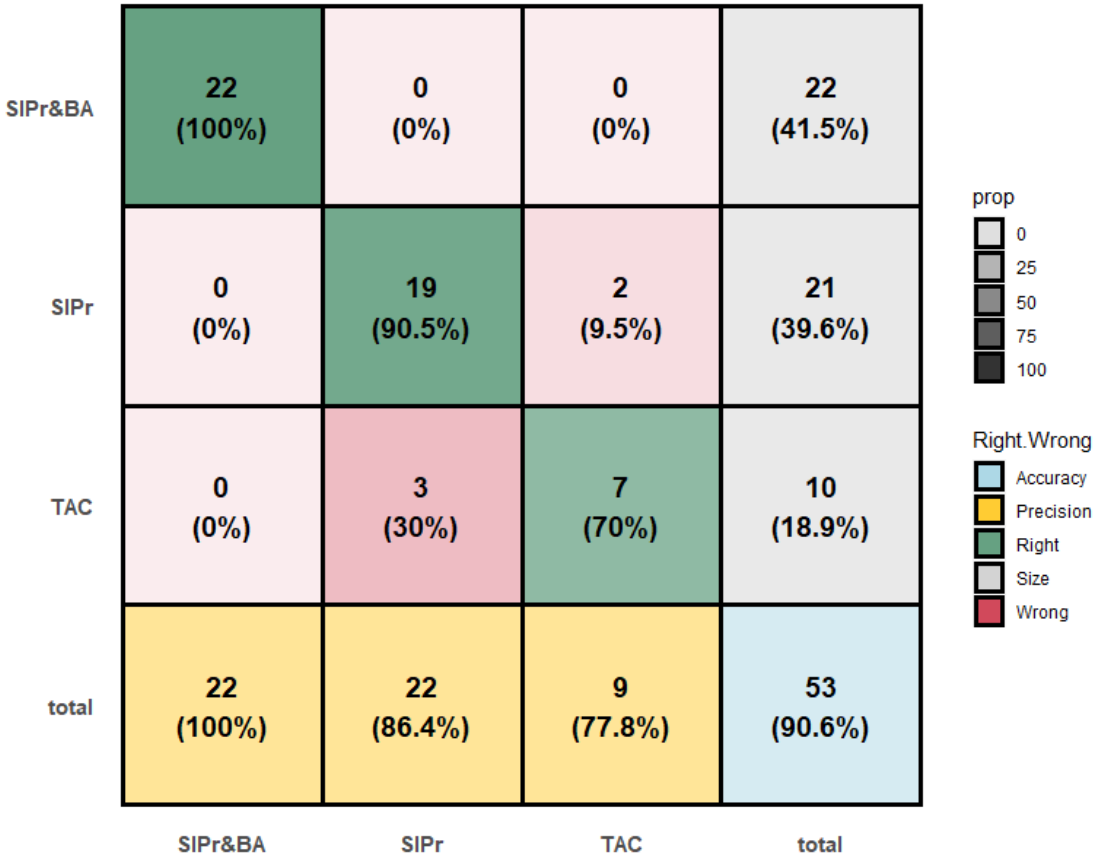
Coefficients

	(Intercept)	C.O	position3	position4	Tot	L	B5
2	-18.58340	-268.1536	187.1947	732.3375	179.7586	-354.0493	540.6776
3	-21.16579	-271.2674	187.3292	176.3736	179.9155	-353.6382	541.3158

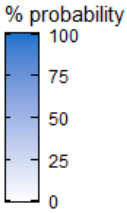
exp(coefficients)

	(Intercept)	C.O	position3	position4	Tot	L	B5

2	0	0	1.984309e+81	Inf	1.169966e+78	0	6.505794e+234
3	0	0	2.269956e+81	3.963499e+76	1.368737e+78	0	1.231634e+235



	SIPr&BA	SIPr	TAC	Exp
2-F	100	0	0	SIPr&BA
3-Br	100	0	0	SIPr&BA
3-Cl	100	0	0	SIPr&BA
3-CN	100	0	0	SIPr&BA
3-F	100	0	0	SIPr&BA
3-I	100	0	0	SIPr&BA
3-CO2Me	100	0	0	SIPr&BA
3-CF3	100	0	0	SIPr&BA
4-Br	100	0	0	SIPr&BA
4-Cl	100	0	0	SIPr&BA
4-CN	100	0	0	SIPr&BA
4-F	100	0	0	SIPr&BA
4-I	100	0	0	SIPr&BA
4-CO2Me	100	0	0	SIPr&BA
4-CF3	100	0	0	SIPr&BA
3,5-Br	100	0	0	SIPr&BA
3,5-Cl	100	0	0	SIPr&BA
6a	100	0	0	SIPr&BA
6b	100	0	0	SIPr&BA
6c	100	0	0	SIPr&BA
6d	100	0	0	SIPr&BA
6e	100	0	0	SIPr&BA
2-Br	0	91	9	SIPr
2-Cl	0	90	10	SIPr
2-C=CH	0	93	7	SIPr
2-OH	0	56	44	SIPr
2-Ome	0	29	71	SIPr
2-Me	0	55	45	SIPr
2-CF3	0	97	3	SIPr
2-OCF3	0	86	14	SIPr
3-Me	0	99	1	SIPr
3-Ome	0	99	1	SIPr
4-CH(OEt)2	0	100	0	SIPr
4-iPr	0	100	0	SIPr
4-Ome	0	100	0	SIPr
4-Me	0	100	0	SIPr
6f	0	85	15	SIPr
6g	0	82	18	SIPr
6h	0	96	4	SIPr
6i	0	96	4	SIPr
6j	0	88	12	SIPr
6k	0	87	13	SIPr
6l	0	48	52	SIPr
6m	0	54	46	TAC
6n	0	10	90	TAC
6o	0	90	10	TAC
6p	0	14	86	TAC
6q	0	70	30	TAC
6r	0	46	54	TAC
6s	0	38	62	TAC
6t	0	2	98	TAC
6u	0	0	100	TAC
6v	0	1	99	TAC



formula = class ~ C=O + position + L + Tot+ B5 + NBO_Carbonyl

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
65.58	81.13	50.94

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	21	1	0	***	SIPr&BA	18	4	0
SIPr	3	15	3	***	SIPr	3	8	10
TAC	0	3	7	***	TAC	0	9	1

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
90.57%	0.82

Variable Importance

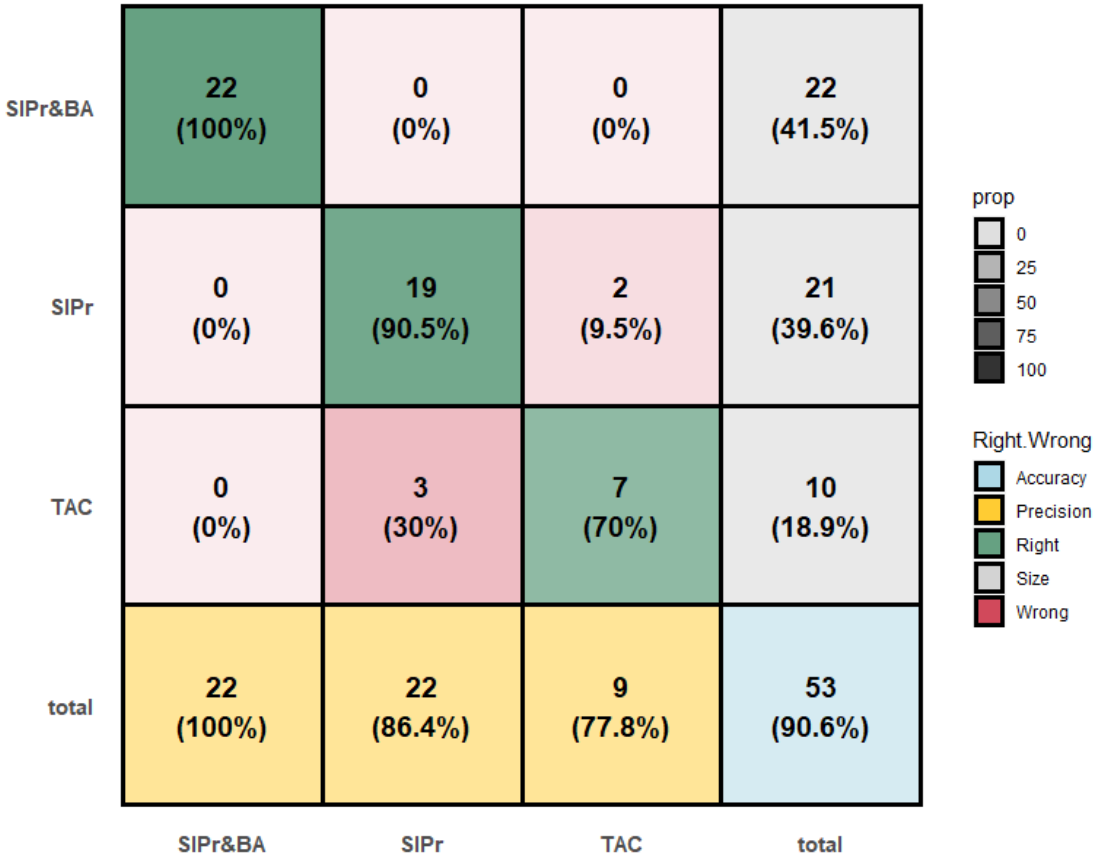
	Overall
C.O	665.7614
L	588.1003
Tot	283.3326
B5	924.4580
position3	120.0546
position4	467.3937
NBO_Carbonyl	451.7816

Coefficients

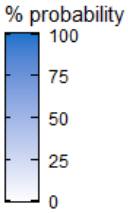
	(Intercept)	C.O	L	Tot	B5	position3	position4	NBO_Carbonyl
2	115.3682	-331.2459	-294.2340	141.6000	461.8662	-60.03250	383.89893	225.7403
3	112.7164	-334.5155	-293.8663	141.7327	462.5917	-60.02211	83.4947	226.0412

exp(coefficients)

	(Intercept)	C.O	L	Tot	B5	position3	position4	NBO_Carbonyl
2	1.269913e+50	0	0	3.133966e+61	3.854349e+200	0	5.311122e+166	1.090901e+98
3	8.955521e+48	0	0	3.578581e+61	7.962377e+200	0	1.825264e+36	1.473896e+98



	SIPr&BA	SIPr	TAC	Exp
2-F	100	0	0	SIPr&BA
3-Br	100	0	0	SIPr&BA
3-Cl	100	0	0	SIPr&BA
3-CN	100	0	0	SIPr&BA
3-F	100	0	0	SIPr&BA
3-I	100	0	0	SIPr&BA
3-CO2Me	100	0	0	SIPr&BA
3-CF3	100	0	0	SIPr&BA
4-Br	100	0	0	SIPr&BA
4-Cl	100	0	0	SIPr&BA
4-CN	100	0	0	SIPr&BA
4-F	100	0	0	SIPr&BA
4-I	100	0	0	SIPr&BA
4-CO2Me	100	0	0	SIPr&BA
4-CF3	100	0	0	SIPr&BA
3,5-Br	100	0	0	SIPr&BA
3,5-Cl	100	0	0	SIPr&BA
6a	100	0	0	SIPr&BA
6b	100	0	0	SIPr&BA
6c	100	0	0	SIPr&BA
6d	100	0	0	SIPr&BA
6e	100	0	0	SIPr&BA
2-Br	0	91	9	SIPr
2-Cl	0	91	9	SIPr
2-C=CH	0	94	6	SIPr
2-OH	0	58	42	SIPr
2-Ome	0	29	71	SIPr
2-Me	0	54	46	SIPr
2-CF3	0	98	2	SIPr
2-OCF3	0	86	14	SIPr
3-Me	0	99	1	SIPr
3-Ome	0	99	1	SIPr
4-CH(OEt)2	0	100	0	SIPr
4-iPr	0	100	0	SIPr
4-Ome	0	100	0	SIPr
4-Me	0	100	0	SIPr
6f	0	86	14	SIPr
6g	0	79	21	SIPr
6h	0	97	3	SIPr
6i	0	96	4	SIPr
6j	0	88	12	SIPr
6k	0	87	13	SIPr
6l	0	47	53	SIPr
6m	0	57	43	TAC
6n	0	8	92	TAC
6o	0	91	9	TAC
6p	0	13	87	TAC
6q	0	67	33	TAC
6r	0	45	55	TAC
6s	0	37	63	TAC
6t	0	4	96	TAC
6u	0	0	100	TAC
6v	0	1	99	TAC



formula = class ~ C=O + L + NBO_Carbonyl

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
63.1	73.58	43.4

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	17	4	1	***	SIPr&BA	10	12	0
SIPr	2	17	2	***	SIPr	6	12	3
TAC	1	4	5	***	TAC	0	9	1

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
69.81%	0.449

Variable Importance

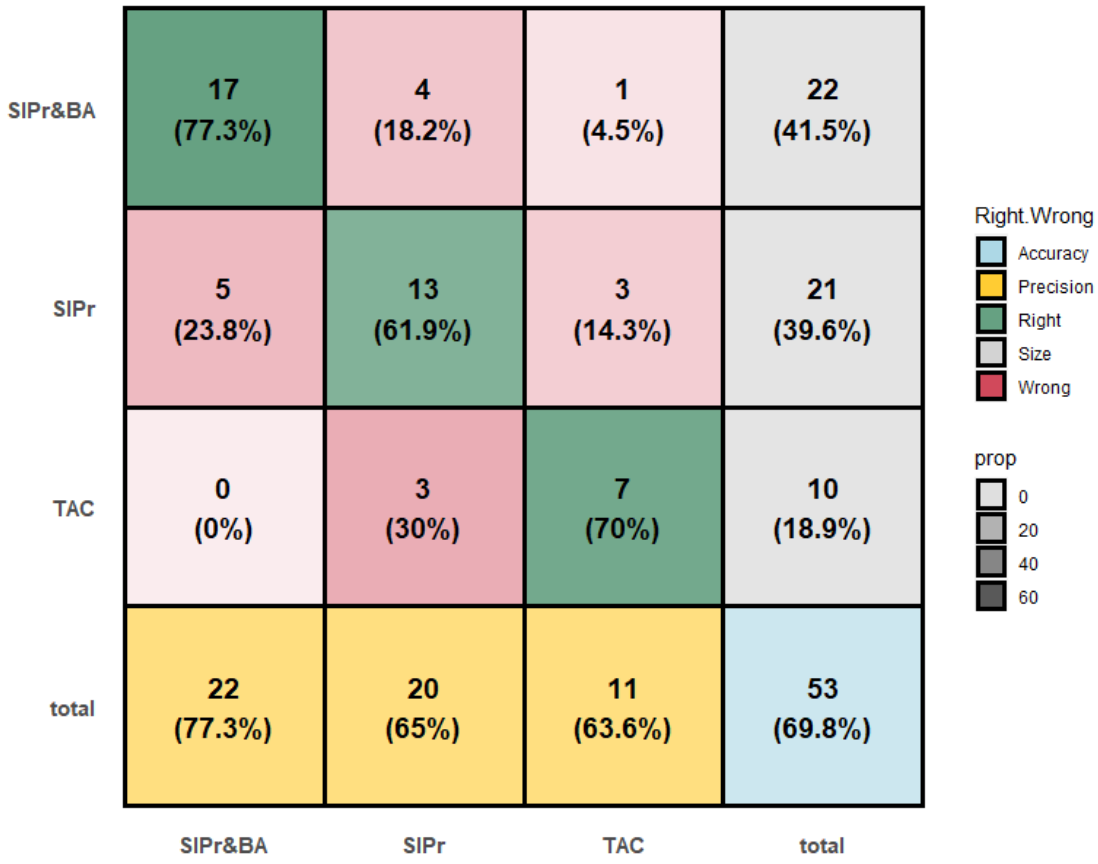
	Overall
C.O	12.733032
L	1.424726
NBO_Carbonyl	5.880758

Coefficients

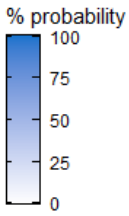
	(Intercept)	C.O	L	NBO_Carbonyl
2	0.9080875	-4.695235	0.3168392	2.949197
3	-1.7178265	-8.037797	1.1078868	2.931560

exp(coefficients)

	(Intercept)	C.O	L	NBO_Carbonyl
2	2.4795758	0.0091387	1.372782	19.09062
3	0.1794558	0.0003230	3.027953	18.75687


SIPr&BA
SIPr
TAC
total
17 (77.3%)
4 (18.2%)
1 (4.5%)
22 (41.5%)
5 (23.8%)
13 (61.9%)
3 (14.3%)
21 (39.6%)
0 (0%)
3 (30%)
7 (70%)
10 (18.9%)
22 (77.3%)
20 (65%)
11 (63.6%)
53 (69.8%)
SIPr&BA
SIPr
TAC
total
Right.Wrong
Accuracy
Precision
Right
Size
Wrong
prop
0
20
40
60

	SIPr&BA	SIPr	TAC	Exp
2-F	27	67	6	SIPr&BA
3-Br	85	15	0	SIPr&BA
3-Cl	86	14	0	SIPr&BA
3-CN	97	3	0	SIPr&BA
3-F	92	8	0	SIPr&BA
3-I	81	19	0	SIPr&BA
3-CO2Me	60	40	0	SIPr&BA
3-CF3	93	7	0	SIPr&BA
4-Br	60	39	0	SIPr&BA
4-Cl	58	42	1	SIPr&BA
4-CN	98	2	0	SIPr&BA
4-F	41	59	1	SIPr&BA
4-I	55	45	1	SIPr&BA
4-CO2Me	87	13	0	SIPr&BA
4-CF3	96	4	0	SIPr&BA
3,5-Br	95	5	0	SIPr&BA
3,5-Cl	96	4	0	SIPr&BA
6a	40	54	6	SIPr&BA
6b	85	15	0	SIPr&BA
6c	59	17	24	SIPr&BA
6d	48	51	1	SIPr&BA
6e	16	25	59	SIPr&BA
2-Br	16	76	8	SIPr
2-Cl	17	74	9	SIPr
2-C=CH	56	41	3	SIPr
2-OH	1	52	47	SIPr
2-Ome	0	33	67	SIPr
2-Me	0	48	51	SIPr
2-CF3	89	10	0	SIPr
2-OCF3	20	71	9	SIPr
3-Me	33	66	1	SIPr
3-Ome	50	50	0	SIPr
4-CH(OEt)2	33	66	2	SIPr
4-iPr	7	86	6	SIPr
4-Ome	1	75	24	SIPr
4-Me	14	83	3	SIPr
6f	83	17	0	SIPr
6g	4	85	10	SIPr
6h	54	45	1	SIPr
6i	49	51	0	SIPr
6j	10	79	11	SIPr
6k	43	54	3	SIPr
6l	1	50	50	SIPr
6m	13	57	30	TAC
6n	0	26	74	TAC
6o	14	79	7	TAC
6p	0	22	78	TAC
6q	1	76	23	TAC
6r	0	39	61	TAC
6s	0	40	60	TAC
6t	36	2	62	TAC
6u	0	0	100	TAC
6v	0	0	100	TAC



formula = class ~ C=O + L + NBO_Carbonyl + B5

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
69.53	84.91	49.06

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	20	2	0	***	SIPr&BA	9	13	0
SIPr	2	18	1	***	SIPr	6	10	5
TAC	0	3	7	***	TAC	0	3	7

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
86.79%	0.628

Variable Importance

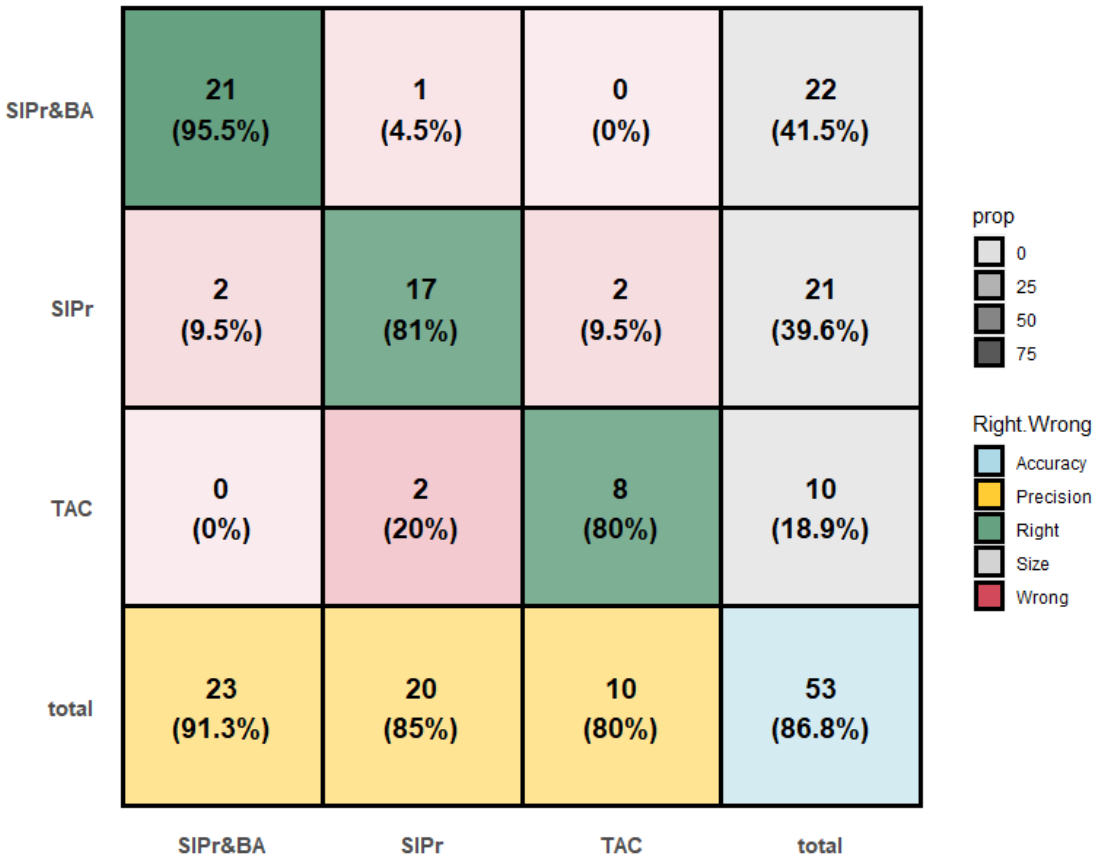
	Overall
C.O	23.054697
L	5.679185
NBO_Carbonyl	13.957159
B5	10.344471

Coefficients

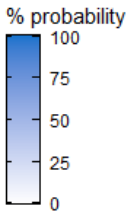
	(Intercept)	C.O	L	NBO_Carbonyl	B5
2	2.7076799	-9.654709	-2.936004	6.836435	4.568646
3	-0.3941922	-13.399988	-2.743182	7.120725	5.775825

exp(coefficients)

	(Intercept)	C.O	L	NBO_Carbonyl	B5
2	14.9944467	6.41e-05	0.0530774	931.1631	96.41347
3	0.6742245	1.50e-06	0.0643652	1237.3473	322.41022


SIPr&BA
SIPr
TAC
total
21 (95.5%)
1 (4.5%)
0 (0%)
22 (41.5%)
2 (9.5%)
17 (81%)
2 (9.5%)
21 (39.6%)
0 (0%)
2 (20%)
8 (80%)
10 (18.9%)
23 (91.3%)
20 (85%)
10 (80%)
53 (86.8%)
SIPr&BA
SIPr
TAC
total
prop
0
25
50
75
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	20	77	3	SIPr&BA
3-Br	81	19	0	SIPr&BA
3-Cl	89	11	0	SIPr&BA
3-CN	99	1	0	SIPr&BA
3-F	99	1	0	SIPr&BA
3-I	66	34	0	SIPr&BA
3-CO2Me	78	22	0	SIPr&BA
3-CF3	96	4	0	SIPr&BA
4-Br	99	1	0	SIPr&BA
4-Cl	99	1	0	SIPr&BA
4-CN	100	0	0	SIPr&BA
4-F	76	23	0	SIPr&BA
4-I	99	1	0	SIPr&BA
4-CO2Me	100	0	0	SIPr&BA
4-CF3	100	0	0	SIPr&BA
3,5-Br	98	2	0	SIPr&BA
3,5-Cl	99	1	0	SIPr&BA
6a	66	30	3	SIPr&BA
6b	76	23	0	SIPr&BA
6c	100	0	0	SIPr&BA
6d	76	23	0	SIPr&BA
6e	63	22	15	SIPr&BA
2-Br	1	93	7	SIPr
2-Cl	2	92	7	SIPr
2-C=CH	11	85	4	SIPr
2-OH	0	65	35	SIPr
2-Ome	0	29	71	SIPr
2-Me	0	57	43	SIPr
2-CF3	96	4	0	SIPr
2-OCF3	0	87	12	SIPr
3-Me	5	95	1	SIPr
3-Ome	33	67	0	SIPr
4-CH(OEt)2	43	56	1	SIPr
4-iPr	39	60	1	SIPr
4-Ome	1	92	6	SIPr
4-Me	24	75	1	SIPr
6f	1	86	13	SIPr
6g	0	74	26	SIPr
6h	52	48	1	SIPr
6i	0	95	5	SIPr
6j	0	90	10	SIPr
6k	0	85	14	SIPr
6l	0	45	55	SIPr
6m	0	49	51	TAC
6n	0	4	96	TAC
6o	0	92	7	TAC
6p	0	10	90	TAC
6q	0	73	27	TAC
6r	0	47	53	TAC
6s	0	45	55	TAC
6t	11	1	88	TAC
6u	0	0	100	TAC
6v	0	0	100	TAC



formula = class ~ C=O + L + B5 + diff_Ca_Cr

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
68.35	81.13	50.94

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	19	3	0	***	SIPr&BA	11	11	0
SIPr	2	18	1	***	SIPr	8	10	3
TAC	0	4	6	***	TAC	0	4	6

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
75.47%	0.533

Variable Importance

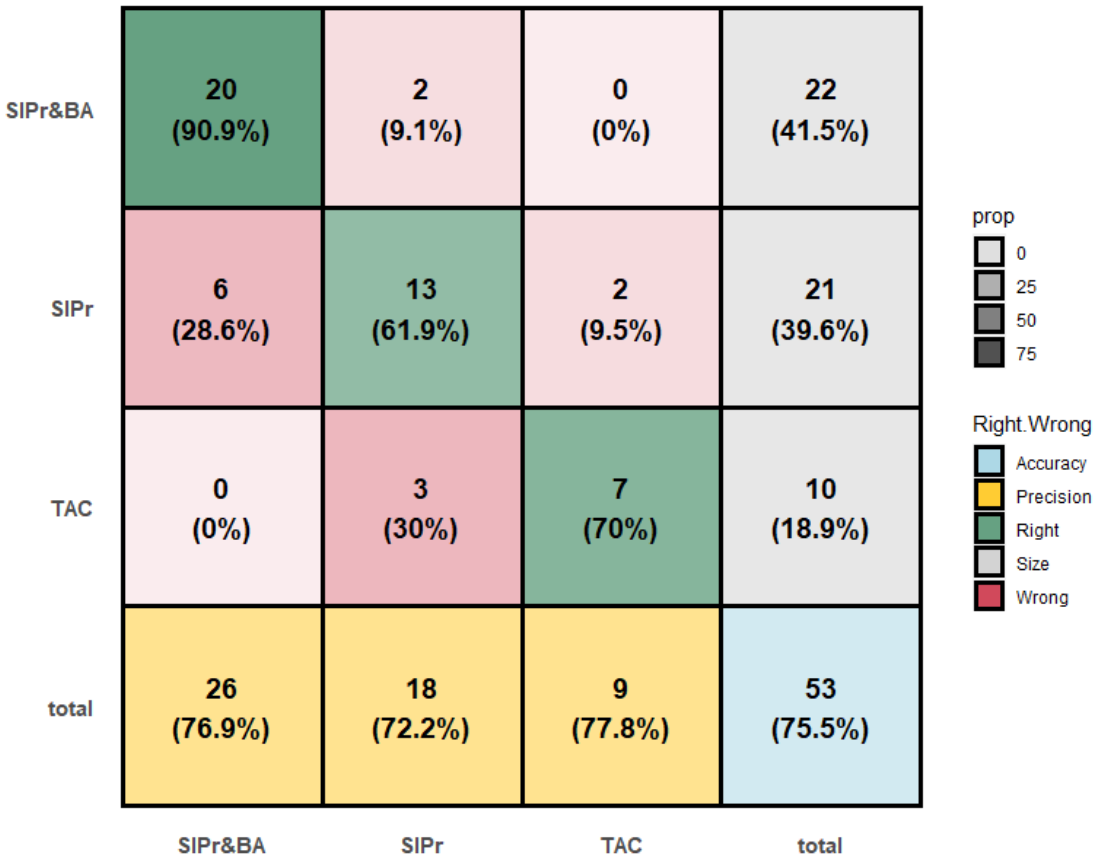
	Overall
C.O	14.1628524
L	0.3586212
B5	3.6137261
diff_Ca_Cr	6.4524757

Coefficients

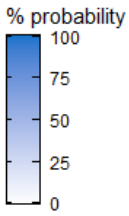
	(Intercept)	C.O	L	B5	diff_Ca_Cr
2	2.5944164	-5.338580	-0.3044727	1.346248	-2.965654
3	-0.2072611	-8.824273	0.0541485	2.267479	-3.486822

exp(coefficients)

	(Intercept)	C.O	L	B5	diff_Ca_Cr
2	13.3887713	0.0048027	0.7375121	3.842978	0.0515268
3	0.8128074	0.0001471	1.0556414	9.655025	0.0305980


SIPr&BA
SIPr
TAC
total
20 (90.9%)
2 (9.1%)
0 (0%)
22 (41.5%)
6 (28.6%)
13 (61.9%)
2 (9.5%)
21 (39.6%)
0 (0%)
3 (30%)
7 (70%)
10 (18.9%)
26 (76.9%)
18 (72.2%)
9 (77.8%)
53 (75.5%)
SIPr&BA
SIPr
TAC
total
prop
0
25
50
75
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	61	38	1	SIPr&BA
3-Br	85	15	0	SIPr&BA
3-Cl	86	14	0	SIPr&BA
3-CN	97	3	0	SIPr&BA
3-F	89	11	0	SIPr&BA
3-I	82	18	0	SIPr&BA
3-CO2Me	84	16	0	SIPr&BA
3-CF3	94	6	0	SIPr&BA
4-Br	90	10	0	SIPr&BA
4-Cl	89	11	0	SIPr&BA
4-CN	96	4	0	SIPr&BA
4-F	89	11	0	SIPr&BA
4-I	89	11	0	SIPr&BA
4-CO2Me	90	10	0	SIPr&BA
4-CF3	97	3	0	SIPr&BA
3,5-Br	92	8	0	SIPr&BA
3,5-Cl	93	7	0	SIPr&BA
6a	35	57	8	SIPr&BA
6b	1	96	4	SIPr&BA
6c	73	23	4	SIPr&BA
6d	69	30	1	SIPr&BA
6e	70	24	6	SIPr&BA
2-Br	9	85	6	SIPr
2-Cl	5	88	7	SIPr
2-C=CH	0	90	10	SIPr
2-OH	1	70	28	SIPr
2-Ome	0	38	62	SIPr
2-Me	0	55	45	SIPr
2-CF3	2	95	3	SIPr
2-OCF3	4	85	11	SIPr
3-Me	50	50	0	SIPr
3-Ome	54	45	0	SIPr
4-CH(OEt)2	55	44	1	SIPr
4-iPr	52	47	1	SIPr
4-Ome	27	68	5	SIPr
4-Me	59	40	0	SIPr
6f	29	63	8	SIPr
6g	0	72	27	SIPr
6h	60	39	1	SIPr
6i	6	90	4	SIPr
6j	9	83	8	SIPr
6k	7	79	14	SIPr
6l	0	39	61	SIPr
6m	0	42	58	TAC
6n	0	9	91	TAC
6o	16	79	5	TAC
6p	0	18	82	TAC
6q	0	70	30	TAC
6r	0	39	61	TAC
6s	1	52	47	TAC
6t	0	0	100	TAC
6u	0	0	100	TAC
6v	0	1	99	TAC



formula = class ~ C=O + L + B5 + NBO_Carbonyl + position

K-Fold CV - 3 folds for 500 iterations

```
Error in rbind(deparse.level, ...): numbers of columns of arguments do
not match
```

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
81.13%	0.655

Variable Importance

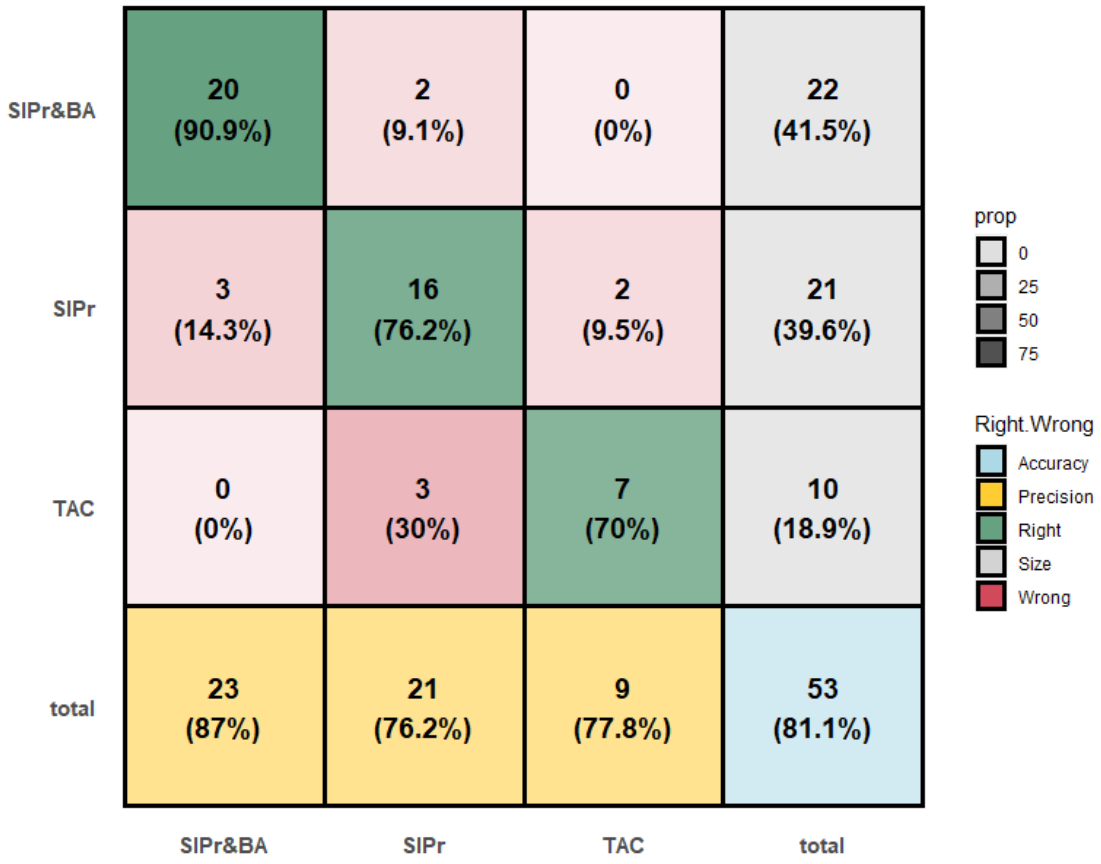
	Overall
C.O	24.0009042
L	9.3924542
B5	16.2021881
NBO_Carbonyl	14.2811948
position3	0.9997513
position4	6.8633465

Coefficients

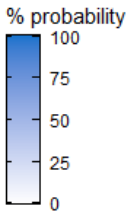
	(Intercept)	C.O	L	B5	NBO_Carbonyl	position3	position4
2	2.3904456	-10.26445	-4.812471	7.659236	6.913275	0.3993959	4.171610
3	-0.4327538	-13.73646	-4.579983	8.542952	7.367920	0.6003554	-2.691737

exp(coefficients)

	(Intercept)	C.O	L	B5	NBO_Carbonyl	position3	position4
2	10.9183578	3.49e-05	0.0081278	2120.138	1005.535	1.490924	64.8197296
3	0.6487202	1.10e-06	0.0102551	5130.465	1584.335	1.822766	0.0677632


SIPr&BA
SIPr
TAC
total
20 (90.9%)
2 (9.1%)
0 (0%)
22 (41.5%)
3 (14.3%)
16 (76.2%)
2 (9.5%)
21 (39.6%)
0 (0%)
3 (30%)
7 (70%)
10 (18.9%)
23 (87%)
21 (76.2%)
9 (77.8%)
53 (81.1%)
SIPr&BA
SIPr
TAC
total
prop
0
25
50
75
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	48	50	3	SIPr&BA
3-Br	84	16	0	SIPr&BA
3-Cl	93	7	0	SIPr&BA
3-CN	99	1	0	SIPr&BA
3-F	100	0	0	SIPr&BA
3-I	66	34	0	SIPr&BA
3-CO2Me	93	7	0	SIPr&BA
3-CF3	97	3	0	SIPr&BA
4-Br	99	1	0	SIPr&BA
4-Cl	98	2	0	SIPr&BA
4-CN	100	0	0	SIPr&BA
4-F	47	53	0	SIPr&BA
4-I	100	0	0	SIPr&BA
4-CO2Me	100	0	0	SIPr&BA
4-CF3	100	0	0	SIPr&BA
3,5-Br	99	1	0	SIPr&BA
3,5-Cl	100	0	0	SIPr&BA
6a	68	28	4	SIPr&BA
6b	65	34	1	SIPr&BA
6c	100	0	0	SIPr&BA
6d	89	10	0	SIPr&BA
6e	83	10	6	SIPr&BA
2-Br	1	91	8	SIPr
2-Cl	2	90	8	SIPr
2-C=CH	5	90	5	SIPr
2-OH	0	62	38	SIPr
2-Ome	0	30	70	SIPr
2-Me	0	54	46	SIPr
2-CF3	96	4	0	SIPr
2-OCF3	0	87	13	SIPr
3-Me	6	93	1	SIPr
3-Ome	53	46	0	SIPr
4-CH(OEt)2	7	93	0	SIPr
4-iPr	38	62	0	SIPr
4-Ome	1	99	0	SIPr
4-Me	10	90	0	SIPr
6f	0	89	11	SIPr
6g	0	75	25	SIPr
6h	54	45	1	SIPr
6i	0	94	6	SIPr
6j	0	88	12	SIPr
6k	0	86	14	SIPr
6l	0	46	54	SIPr
6m	0	57	43	TAC
6n	0	7	93	TAC
6o	0	91	9	TAC
6p	0	13	87	TAC
6q	0	69	31	TAC
6r	0	46	54	TAC
6s	0	38	62	TAC
6t	0	6	94	TAC
6u	0	0	100	TAC
6v	0	1	99	TAC



formula = class ~ C=O + L + B5

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
64.1	71.7	49.06

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	18	3	1	***	SIPr&BA	15	7	0
SIPr	6	14	1	***	SIPr	7	6	8
TAC	0	4	6	***	TAC	0	5	5

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
67.92%	0.44

Variable Importance

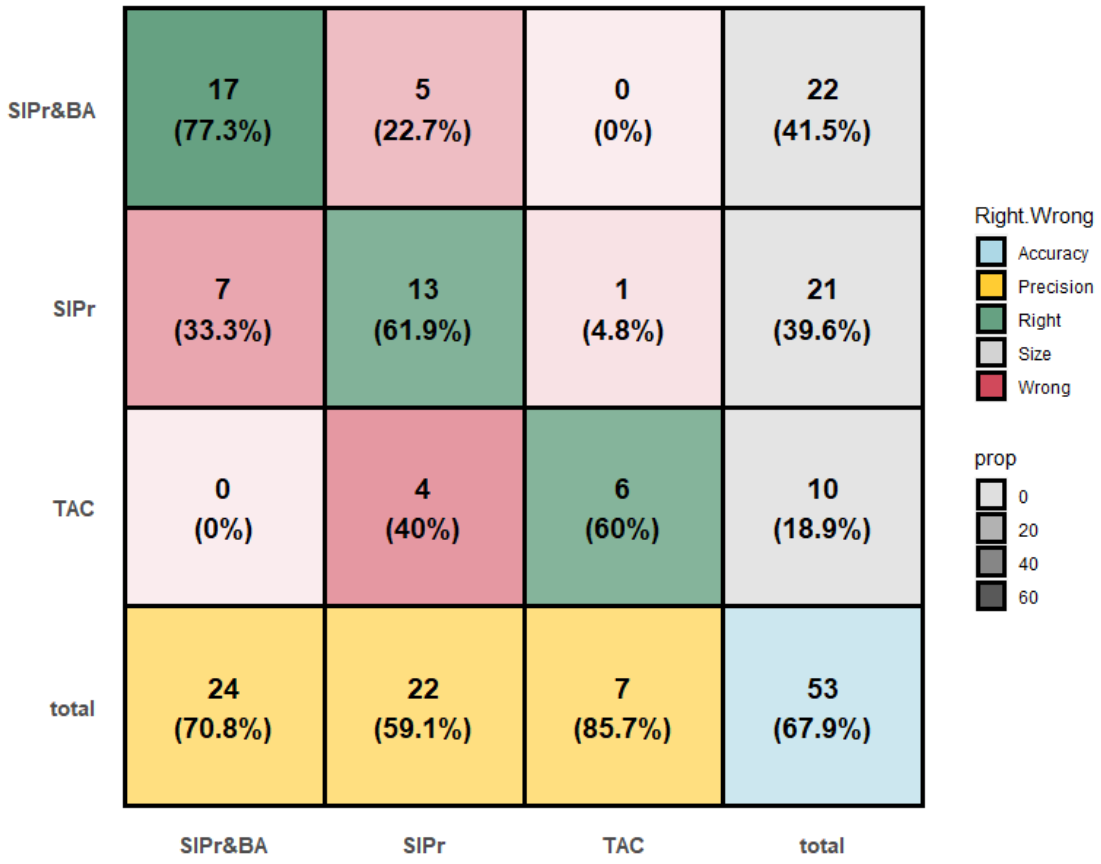
	Overall
C.O	7.199703
L	1.299735
B5	4.234353

Coefficients

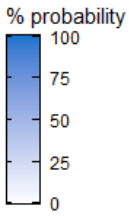
	(Intercept)	C.O	L	B5
2	0.7996756	-2.039869	-0.7006940	1.523480
3	-2.0641716	-5.159834	-0.5990407	2.710872

exp(coefficients)

	(Intercept)	C.O	L	B5
2	2.2248192	0.1300458	0.4962408	4.588166
3	0.1269234	0.0057427	0.5493384	15.042391


SIPr&BA
SIPr
TAC
total
17 (77.3%)
5 (22.7%)
0 (0%)
22 (41.5%)
7 (33.3%)
13 (61.9%)
1 (4.8%)
21 (39.6%)
0 (0%)
4 (40%)
6 (60%)
10 (18.9%)
24 (70.8%)
22 (59.1%)
7 (85.7%)
53 (67.9%)
SIPr&BA
SIPr
TAC
total
Right.Wrong
Accuracy
Precision
Right
Size
Wrong
prop
0
20
40
60

	SIPr&BA	SIPr	TAC	Exp
2-F	35	62	3	SIPr&BA
3-Br	75	25	0	SIPr&BA
3-Cl	78	22	0	SIPr&BA
3-CN	81	19	0	SIPr&BA
3-F	86	14	0	SIPr&BA
3-I	71	29	0	SIPr&BA
3-CO2Me	74	26	0	SIPr&BA
3-CF3	78	22	0	SIPr&BA
4-Br	89	11	0	SIPr&BA
4-Cl	86	14	0	SIPr&BA
4-CN	96	4	0	SIPr&BA
4-F	79	21	0	SIPr&BA
4-I	89	10	0	SIPr&BA
4-CO2Me	95	5	0	SIPr&BA
4-CF3	95	5	0	SIPr&BA
3,5-Br	85	15	0	SIPr&BA
3,5-Cl	87	13	0	SIPr&BA
6a	42	52	7	SIPr&BA
6b	34	65	2	SIPr&BA
6c	21	61	18	SIPr&BA
6d	64	35	1	SIPr&BA
6e	4	53	43	SIPr&BA
2-Br	20	74	6	SIPr
2-Cl	21	73	6	SIPr
2-C=CH	18	76	6	SIPr
2-OH	7	64	29	SIPr
2-Ome	1	36	63	SIPr
2-Me	6	60	34	SIPr
2-CF3	36	62	2	SIPr
2-OCF3	10	77	13	SIPr
3-Me	59	41	0	SIPr
3-Ome	71	29	0	SIPr
4-CH(OEt)2	65	34	0	SIPr
4-iPr	76	23	0	SIPr
4-Ome	55	43	2	SIPr
4-Me	72	28	0	SIPr
6f	8	75	17	SIPr
6g	4	72	25	SIPr
6h	55	44	1	SIPr
6i	4	88	8	SIPr
6j	15	75	9	SIPr
6k	12	73	15	SIPr
6l	2	50	48	SIPr
6m	1	47	52	TAC
6n	0	6	94	TAC
6o	17	76	7	TAC
6p	0	15	85	TAC
6q	7	71	22	TAC
6r	5	52	43	TAC
6s	7	52	41	TAC
6t	0	1	99	TAC
6u	0	0	100	TAC
6v	0	1	99	TAC



formula = class ~ C=O + L + NBO_Carbonyl

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
62.95	75.47	50.94

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	19	3	0	***	SIPr&BA	13	8	1
SIPr	5	15	1	***	SIPr	7	10	4
TAC	1	3	6	***	TAC	1	5	4

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
69.81%	0.449

Variable Importance

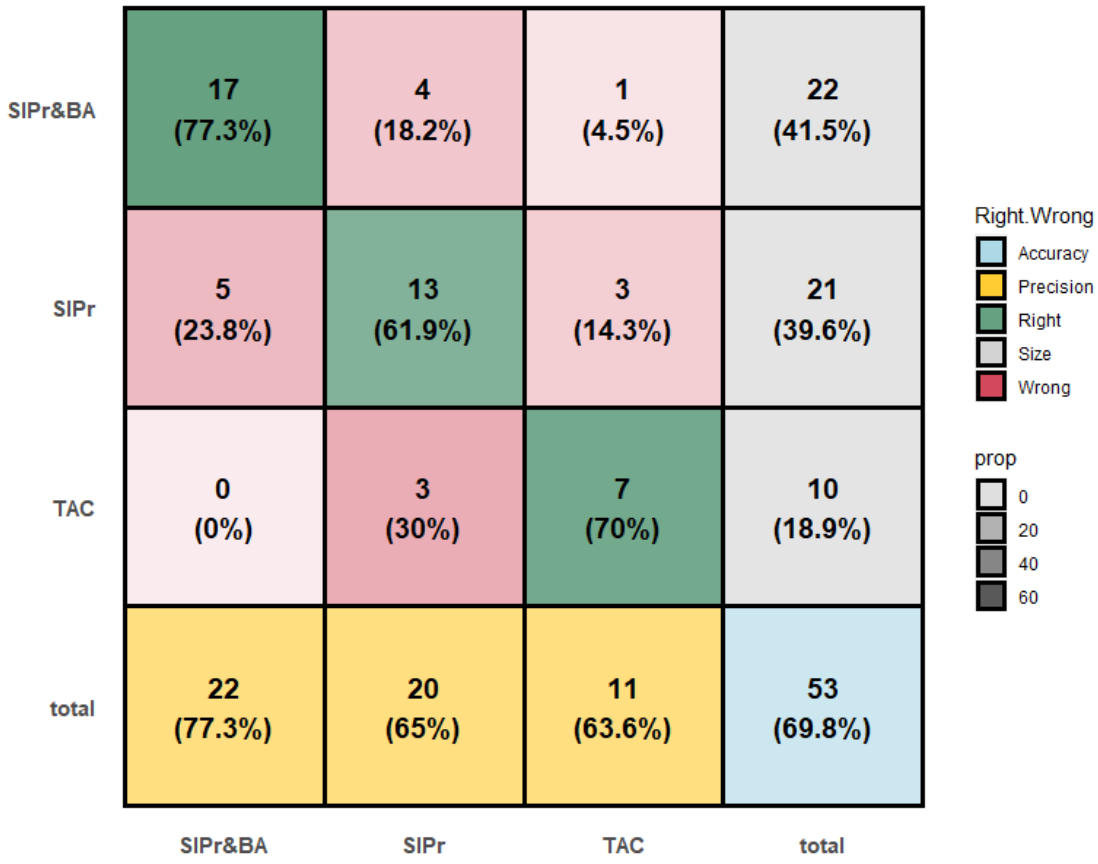
	Overall
C.O	12.733032
L	1.424726
NBO_Carbonyl	5.880758

Coefficients

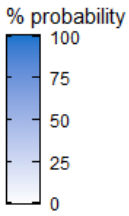
	(Intercept)	C.O	L	NBO_Carbonyl
2	0.9080875	-4.695235	0.3168392	2.949197
3	-1.7178265	-8.037797	1.1078868	2.931560

exp(coefficients)

	(Intercept)	C.O	L	NBO_Carbonyl
2	2.4795758	0.0091387	1.372782	19.09062
3	0.1794558	0.0003230	3.027953	18.75687


SIPr&BA
SIPr
TAC
total
17 (77.3%)
4 (18.2%)
1 (4.5%)
22 (41.5%)
5 (23.8%)
13 (61.9%)
3 (14.3%)
21 (39.6%)
0 (0%)
3 (30%)
7 (70%)
10 (18.9%)
22 (77.3%)
20 (65%)
11 (63.6%)
53 (69.8%)
SIPr&BA
SIPr
TAC
total
Right.Wrong
Accuracy
Precision
Right
Size
Wrong
prop
0
20
40
60

	SIPr&BA	SIPr	TAC	Exp
2-F	27	67	6	SIPr&BA
3-Br	85	15	0	SIPr&BA
3-Cl	86	14	0	SIPr&BA
3-CN	97	3	0	SIPr&BA
3-F	92	8	0	SIPr&BA
3-I	81	19	0	SIPr&BA
3-CO2Me	60	40	0	SIPr&BA
3-CF3	93	7	0	SIPr&BA
4-Br	60	39	0	SIPr&BA
4-Cl	58	42	1	SIPr&BA
4-CN	98	2	0	SIPr&BA
4-F	41	59	1	SIPr&BA
4-I	55	45	1	SIPr&BA
4-CO2Me	87	13	0	SIPr&BA
4-CF3	96	4	0	SIPr&BA
3,5-Br	95	5	0	SIPr&BA
3,5-Cl	96	4	0	SIPr&BA
6a	40	54	6	SIPr&BA
6b	85	15	0	SIPr&BA
6c	59	17	24	SIPr&BA
6d	48	51	1	SIPr&BA
6e	16	25	59	SIPr&BA
2-Br	16	76	8	SIPr
2-Cl	17	74	9	SIPr
2-C=CH	56	41	3	SIPr
2-OH	1	52	47	SIPr
2-Ome	0	33	67	SIPr
2-Me	0	48	51	SIPr
2-CF3	89	10	0	SIPr
2-OCF3	20	71	9	SIPr
3-Me	33	66	1	SIPr
3-Ome	50	50	0	SIPr
4-CH(OEt)2	33	66	2	SIPr
4-iPr	7	86	6	SIPr
4-Ome	1	75	24	SIPr
4-Me	14	83	3	SIPr
6f	83	17	0	SIPr
6g	4	85	10	SIPr
6h	54	45	1	SIPr
6i	49	51	0	SIPr
6j	10	79	11	SIPr
6k	43	54	3	SIPr
6l	1	50	50	SIPr
6m	13	57	30	TAC
6n	0	26	74	TAC
6o	14	79	7	TAC
6p	0	22	78	TAC
6q	1	76	23	TAC
6r	0	39	61	TAC
6s	0	40	60	TAC
6t	36	2	62	TAC
6u	0	0	100	TAC
6v	0	0	100	TAC



formula = class ~ C=O + L + B1 + NBO_Carbonyl

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
62.06	75.47	47.17

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	20	1	1	***	SIPr&BA	15	7	0
SIPr	5	13	3	***	SIPr	6	8	7
TAC	1	2	7	***	TAC	1	7	2

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
73.58%	0.497

Variable Importance

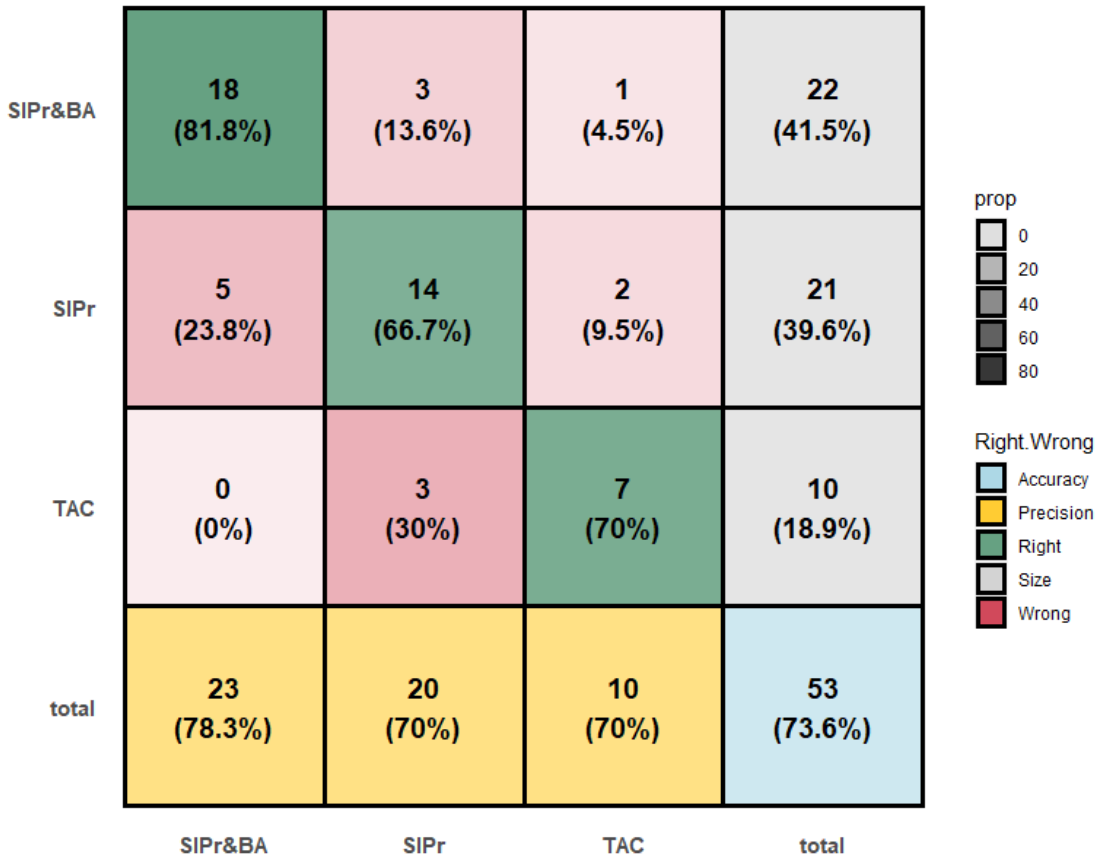
	Overall
C.O	14.503287
L	1.446119
B1	3.107568
NBO_Carbonyl	6.265602

Coefficients

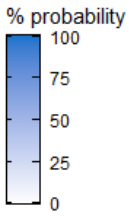
	(Intercept)	C.O	L	B1	NBO_Carbonyl
2	1.125195	-5.351334	0.3210923	1.309060	3.070819
3	-1.733410	-9.151953	1.1250263	1.798509	3.194783

exp(coefficients)

	(Intercept)	C.O	L	B1	NBO_Carbonyl
2	3.0808168	0.0047418	1.378633	3.702690	21.55956
3	0.1766808	0.0001060	3.080298	6.040633	24.40487


SIPr&BA
SIPr
TAC
total
18 (81.8%)
3 (13.6%)
1 (4.5%)
22 (41.5%)
5 (23.8%)
14 (66.7%)
2 (9.5%)
21 (39.6%)
0 (0%)
3 (30%)
7 (70%)
10 (18.9%)
23 (78.3%)
20 (70%)
10 (70%)
53 (73.6%)
SIPr&BA
SIPr
TAC
total
prop
0
20
40
60
80
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	40	57	3	SIPr&BA
3-Br	92	8	0	SIPr&BA
3-Cl	95	5	0	SIPr&BA
3-CN	99	1	0	SIPr&BA
3-F	98	2	0	SIPr&BA
3-I	85	15	0	SIPr&BA
3-CO2Me	77	23	0	SIPr&BA
3-CF3	91	9	0	SIPr&BA
4-Br	44	55	1	SIPr&BA
4-Cl	64	35	0	SIPr&BA
4-CN	99	1	0	SIPr&BA
4-F	63	37	0	SIPr&BA
4-I	12	86	2	SIPr&BA
4-CO2Me	91	9	0	SIPr&BA
4-CF3	82	18	0	SIPr&BA
3,5-Br	94	6	0	SIPr&BA
3,5-Cl	98	2	0	SIPr&BA
6a	63	35	2	SIPr&BA
6b	93	6	0	SIPr&BA
6c	73	14	13	SIPr&BA
6d	63	37	1	SIPr&BA
6e	21	29	50	SIPr&BA
2-Br	16	78	6	SIPr
2-Cl	23	71	6	SIPr
2-C=CH	72	27	1	SIPr
2-OH	1	57	42	SIPr
2-Ome	0	32	68	SIPr
2-Me	0	49	51	SIPr
2-CF3	80	19	0	SIPr
2-OCF3	10	79	10	SIPr
3-Me	44	55	0	SIPr
3-Ome	63	37	0	SIPr
4-CH(OEt)2	0	79	21	SIPr
4-iPr	1	89	10	SIPr
4-Ome	1	77	22	SIPr
4-Me	13	85	2	SIPr
6f	64	35	1	SIPr
6g	7	86	7	SIPr
6h	65	35	0	SIPr
6i	18	81	1	SIPr
6j	12	80	8	SIPr
6k	33	65	3	SIPr
6l	1	54	45	SIPr
6m	2	55	43	TAC
6n	0	24	76	TAC
6o	9	84	7	TAC
6p	0	16	84	TAC
6q	1	80	19	TAC
6r	0	43	56	TAC
6s	0	33	66	TAC
6t	27	2	71	TAC
6u	0	0	100	TAC
6v	0	0	100	TAC



formula = class ~ C=O + B5 + B1 + NBO_Carbonyl

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
66.5	79.25	50.94

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	19	3	0	***	SIPr&BA	13	9	0
SIPr	3	17	1	***	SIPr	4	9	8
TAC	1	3	6	***	TAC	1	4	5

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
75.47%	0.596

Variable Importance

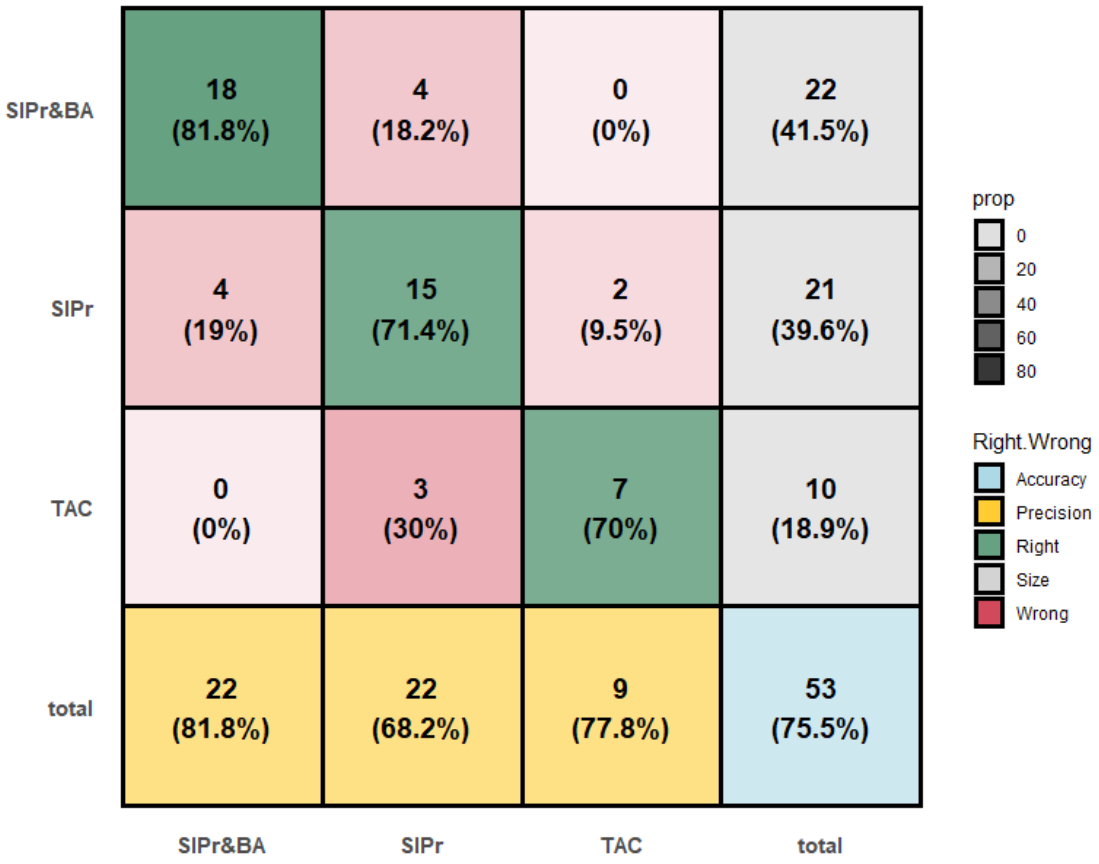
	Overall
C.O	18.219257
B5	3.905848
B1	3.091919
NBO_Carbonyl	8.403939

Coefficients

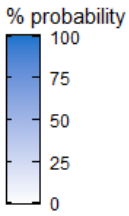
	(Intercept)	C.O	B5	B1	NBO_Carbonyl
2	1.555599	-7.023669	1.306612	1.282730	3.887976
3	-1.765359	-11.195588	2.599236	1.809189	4.515963

exp(coefficients)

	(Intercept)	C.O	B5	B1	NBO_Carbonyl
2	4.7379257	0.0008906	3.693638	3.606472	48.81199
3	0.1711254	0.0000137	13.453454	6.105492	91.46561


SIPr&BA
SIPr
TAC
total
18 (81.8%)
4 (18.2%)
0 (0%)
22 (41.5%)
4 (19%)
15 (71.4%)
2 (9.5%)
21 (39.6%)
0 (0%)
3 (30%)
7 (70%)
10 (18.9%)
22 (81.8%)
22 (68.2%)
9 (77.8%)
53 (75.5%)
SIPr&BA
SIPr
TAC
total
prop
0
20
40
60
80
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	44	54	1	SIPr&BA
3-Br	96	4	0	SIPr&BA
3-Cl	98	2	0	SIPr&BA
3-CN	100	0	0	SIPr&BA
3-F	99	1	0	SIPr&BA
3-I	90	10	0	SIPr&BA
3-CO2Me	84	16	0	SIPr&BA
3-CF3	97	3	0	SIPr&BA
4-Br	79	21	0	SIPr&BA
4-Cl	88	12	0	SIPr&BA
4-CN	100	0	0	SIPr&BA
4-F	82	18	0	SIPr&BA
4-I	41	59	0	SIPr&BA
4-CO2Me	99	1	0	SIPr&BA
4-CF3	98	2	0	SIPr&BA
3,5-Br	98	2	0	SIPr&BA
3,5-Cl	100	0	0	SIPr&BA
6a	27	71	2	SIPr&BA
6b	94	6	0	SIPr&BA
6c	93	7	1	SIPr&BA
6d	52	48	0	SIPr&BA
6e	37	46	17	SIPr&BA
2-Br	9	86	5	SIPr
2-Cl	16	80	4	SIPr
2-C=CH	63	36	1	SIPr
2-OH	0	70	30	SIPr
2-Ome	0	27	73	SIPr
2-Me	0	57	43	SIPr
2-CF3	88	12	0	SIPr
2-OCF3	4	83	13	SIPr
3-Me	47	53	0	SIPr
3-Ome	72	28	0	SIPr
4-CH(OEt)2	0	88	12	SIPr
4-iPr	2	96	2	SIPr
4-Ome	1	94	5	SIPr
4-Me	21	78	1	SIPr
6f	8	82	10	SIPr
6g	1	77	22	SIPr
6h	50	50	0	SIPr
6i	1	89	10	SIPr
6j	5	87	7	SIPr
6k	3	86	11	SIPr
6l	0	49	51	SIPr
6m	0	38	62	TAC
6n	0	3	97	TAC
6o	4	89	7	TAC
6p	0	7	93	TAC
6q	0	74	26	TAC
6r	0	55	44	TAC
6s	0	40	60	TAC
6t	9	3	87	TAC
6u	0	0	100	TAC
6v	0	0	100	TAC



formula = class ~ C=O + L + B1 + NBO_Carbonyl + B5

K-Fold CV - 3 folds for 500 iterations

over.all.accuracy	best	worst
68.52	83.02	49.06

Best (left) and Worst (right) Classification Tables

actual	SIPr&BA	SIPr	TAC		actual	SIPr&BA	SIPr	TAC
SIPr&BA	20	2	0	***	SIPr&BA	13	9	0
SIPr	1	18	2	***	SIPr	4	8	9
TAC	0	4	6	***	TAC	0	5	5

Entire set model - accuracy, classification table and probabilities heatmap

Accuracy	McFadden_R2
90.57%	0.809

Variable Importance

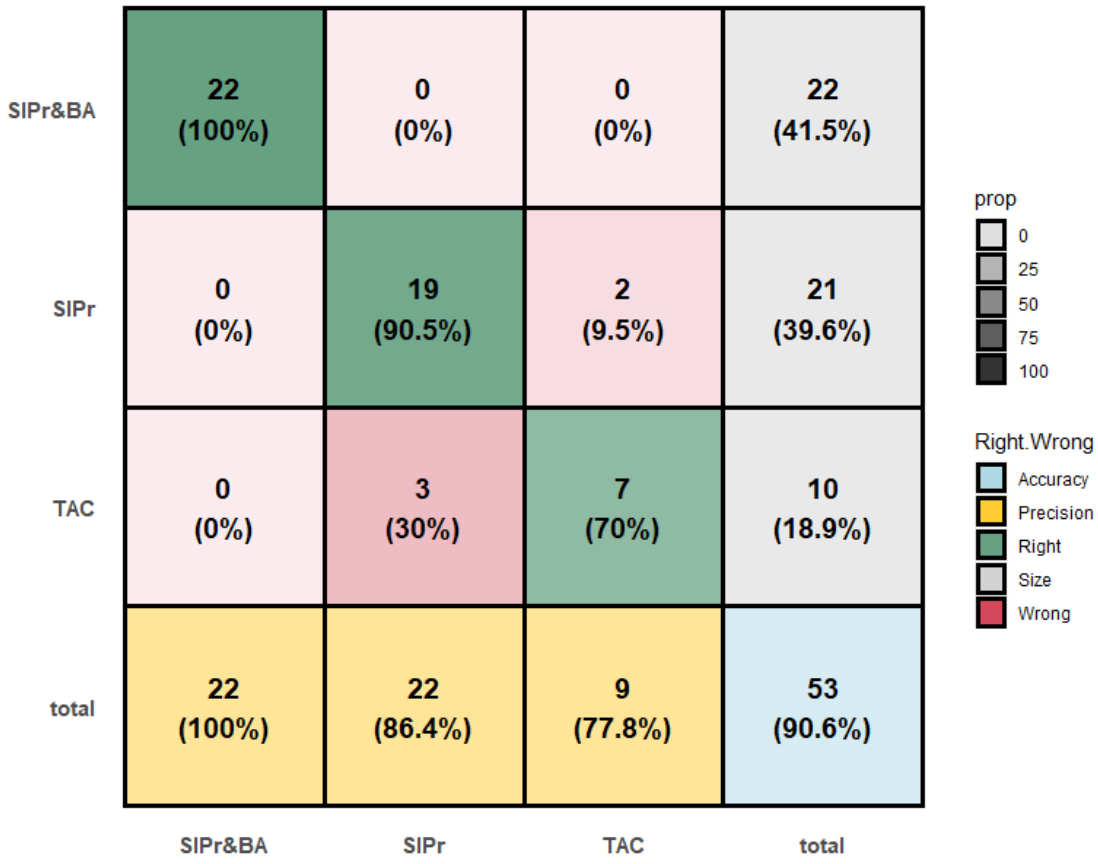
	Overall
C.O	924.1644
L	294.9782
B1	302.2401
NBO_Carbonyl	583.7385
B5	526.7970

Coefficients

	(Intercept)	C.O	L	B1	NBO_Carbonyl	B5
2	181.6280	-460.1144	-147.5902	150.8955	291.6054	262.8799
3	178.5556	-464.0500	-147.3881	151.3446	292.1331	263.9171

exp(coefficients)

	(Intercept)	C.O	L	B1	NBO_Carbonyl	B5
2	7.586391e+78	0	0	3.412492e+65	4.391648e+126	1.469973e+114
3	3.513215e+77	0	0	5.347424e+65	7.443681e+126	4.146990e+114


SIPr&BA
SIPr
TAC
total
22 (100%)
0 (0%)
0 (0%)
22 (41.5%)
0 (0%)
19 (90.5%)
2 (9.5%)
21 (39.6%)
0 (0%)
3 (30%)
7 (70%)
10 (18.9%)
22 (100%)
22 (86.4%)
9 (77.8%)
53 (90.6%)
SIPr&BA
SIPr
TAC
total
prop
0
25
50
75
100
Right.Wrong
Accuracy
Precision
Right
Size
Wrong

	SIPr&BA	SIPr	TAC	Exp
2-F	91	9	0	SIPr&BA
3-Br	100	0	0	SIPr&BA
3-Cl	100	0	0	SIPr&BA
3-CN	100	0	0	SIPr&BA
3-F	100	0	0	SIPr&BA
3-I	82	18	0	SIPr&BA
3-CO2Me	100	0	0	SIPr&BA
3-CF3	100	0	0	SIPr&BA
4-Br	100	0	0	SIPr&BA
4-Cl	100	0	0	SIPr&BA
4-CN	100	0	0	SIPr&BA
4-F	100	0	0	SIPr&BA
4-I	98	2	0	SIPr&BA
4-CO2Me	100	0	0	SIPr&BA
4-CF3	100	0	0	SIPr&BA
3,5-Br	100	0	0	SIPr&BA
3,5-Cl	100	0	0	SIPr&BA
6a	99	1	0	SIPr&BA
6b	100	0	0	SIPr&BA
6c	100	0	0	SIPr&BA
6d	100	0	0	SIPr&BA
6e	100	0	0	SIPr&BA
2-Br	0	93	7	SIPr
2-Cl	0	94	6	SIPr
2-C=CH	0	97	3	SIPr
2-OH	0	67	33	SIPr
2-Ome	0	28	72	SIPr
2-Me	0	55	45	SIPr
2-CF3	7	91	1	SIPr
2-OCF3	0	86	14	SIPr
3-Me	0	99	1	SIPr
3-Ome	22	77	0	SIPr
4-CH(OEt)2	0	88	12	SIPr
4-iPr	0	97	3	SIPr
4-Ome	0	92	8	SIPr
4-Me	0	99	1	SIPr
6f	0	89	11	SIPr
6g	0	80	20	SIPr
6h	0	99	1	SIPr
6i	0	93	7	SIPr
6j	0	91	9	SIPr
6k	0	88	12	SIPr
6l	0	49	51	SIPr
6m	0	43	57	TAC
6n	0	5	95	TAC
6o	0	92	8	TAC
6p	0	9	91	TAC
6q	0	74	26	TAC
6r	0	51	49	TAC
6s	0	37	63	TAC
6t	0	4	96	TAC
6u	0	0	100	TAC
6v	0	0	100	TAC